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FISCAL YEAR 1985 DEPARTMENT OF ENERGY AUTHORIZATION

(Supporting Research and Technical Analysis)

HEARING

BEFORE THE

SUBCOMMITTEE ON
ENERGY DEVELOPMENT AND APPLICATIONS

OF THE

COMMITTEE ON
SCIENCE AND TECHNOLOGY
U.S. HOUSE OF REPRESENTATIVES

NINETY-EIGHTH CONGRESS

SECOND SESSION

FEBRUARY 23, 1984

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Robert S. Kripowicz, *Staff Director*
Harlan L. Watson, *Technical Consultant*

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FISCAL YEAR 1985
DEPARTMENT OF ENERGY
AUTHORIZATION

THURSDAY, FEBRUARY 23, 1984

House of Representatives,
Committee on Science and Technology,
Subcommittee on Energy Development and Applications,
Washington, DC.

The subcommittee met, pursuant to adjournment, at 9:30 a.m., in room 2318, Rayburn House Office Building, Hon. Don Fuqua (chairman of the committee) presiding.

Present: Representatives Fuqua, Harkin, Mineta, Winn, Sensenbrenner, Schneider, Bateman, Lewis, and Gregg.

Staff present: Dr. Harlan L. Watson, technical consultant; and William T. Harvey, minority energy coordinator.

Mr. **Fuqua**. The subcommittee will be in order. This morning, the subcommittee continues its review of the fiscal year 1985 budget request for the Department of Energy's basic research programs. The lead witness again will be Dr. Trivelpiece, accompanied by Dr. Kropschot from DOE's Office of Energy Research to discuss the supporting research and technical analysis programs, which are requesting a total of $480 million in fiscal year 1985, an increase of about $83.6 million or approximately 21 percent above last year's appropriation.

Following the DOE witnesses, we will first hear from Prof. George Pimental from the University of California at Berkeley about current research opportunities in chemical sciences, and then from two distinguished panels composed of university, laboratory, and industrial scientists. At this time, we would like to hear from you, Dr. Trivelpiece. Again, if you wish to summarize your statement, we will place the entire text into the record.

STATEMENT OF DR. ALVIN TRIVELPIECE, DIRECTOR, OFFICE OF ENERGY RESEARCH, U.S. DEPARTMENT OF ENERGY, ACCOMPANIED BY RICHARD H. KROPSCHOT, ASSOCIATE DIRECTOR, OFFICE OF BASIC ENERGY SCIENCES, DOE; AND ANTOINETTE JOSEPH, DIRECTOR, OFFICE OF FIELD OPERATIONS MANAGEMENT, DOE

Dr. **Trivelpiece**. It is good to see you again this morning. I would like to pick up on a slightly different subject.

Yesterday, we talked about the philosophical aspects of how curiosity has caused people over the years to want to know what was in the next valley and across oceans. That curiosity is a natural antecedent of the pure science that we were talking about yesterday. Today, I would like to pick up a different aspect of DOE's activities. It still involves big facilities, but whereas yesterday we were talking about big facilities for big science—in which case, there were detectors and collections of people who are working together that would lead to papers that sometimes have as many as 50 authors on them—we are talking today about the small science that is done on big facilities.

DOE is one of the principal suppliers of big facilities that are used by a large number of scientists in the United States. There is always some sort of a tedious kind of debate that takes place in the area of what is basic science and what is applied science. I will not bore you with the tedious aspects of that debate. More appropriate, I think, is to ask what is appropriate to DOE's mission, and are the things that DOE is doing of high excellence.

In that regard, DOE does not have an educational mission, but yesterday we talked about the need to train people and how DOE's activities fit into that. I would like to begin on that theme this morning.

Without a direct educational mission, nevertheless, DOE, through its contractor activities, supports something in excess of 5,000 graduate students in various areas of the physical sciences in chemistry and mathematics and the like. The people who make up the DOE laboratory staff and many of the contractors, of course, in universities have a direct interest, but many of our laboratories have a rather sincere interest in seeing to it that the talent of our Nation is trained in a way that is appropriate to meet our national needs.

This sincere interest in that kind of training has led our laboratories to do some things, and some of the first things I am going to talk about basically do not cost us anything in Government. The Fermi laboratory—and yesterday you heard from Dr. Lederman, who is the director of that laboratory—started a program about 4 years ago for science for high school students. They do this on a volunteer basis. We provide them a small amount of operating funds for some of the miscellaneous expenses attached to that. But in the past few years, 900 high school students in the Chicago area have spent some 10 Saturdays in different groups learning about quarks, leptons, and various aspects of high energy and nuclear physics and basic science.

I think this is a remarkable contribution these people make, and in fact I would like to acknowledge that the Aurora Foundation in the Illinois area has provided $12,800 to the Friends of Fermilab to continue this excellent volunteer effort. So at that end of the spectrum, we are involved in the training of the next generation of scientists through helping high school students get more acquainted with the science that is practiced by some of our leading scientists.

The university instrumentation program, which is one of the initiatives last year that we talked about, where the loss of good equipment to universities over the years through deterioration and so on, led to a situation in which there was a rather severe shortage—and it persists still—for certain classes of instruments to be used by scientists at academic institutions. We requested last year some $6 million, and $4 million of that survived the process up here. This year we are requesting $6 million again, and we believe this is an important program to help universities in their need to refurbish the equipment that they have.

This year, there is a request for some additional $3 million for the laboratory cooperative program. The collection of DOE's laboratories are a remarkable training ground. They are used as a training ground in some areas for high school students, undergraduate students, and their faculty advisors to spend various periods of time during academic years and during the summer to go there and work at the laboratories. I think this is an excellent activity.

Another small program, which does not involve a great deal of funds, is the so-called PREP program, the prefreshman program. It is primarily for minorities and women. Over the past few years, something like 1,500 women and minority students participate in this program each year. Of them, 75 percent go on to college. In addition to that, there is an apprenticeship program in which minority students can come to the DOE laboratories and work in various areas of science. Some 90 percent of the 300 of them go on to college.

These things are things that I end up discussing on a regular basis in an activity that is called the energy update program. It is made available through a WATS line for radio stations throughout the United States. I have become a regular contributor to that, and I use these subjects of our involvement in education and the use of our laboratories as educational tools on them. I would be glad to supply some of the texts of those scripts for you, if you would be interested in them.

[The material referred to follows:]

ENERGY UPDATE FEATURE PROGRAMS WITH DR. ALVIN TRIVELPIECE

1.	September 2, 1983	Energy Research Activities of DOE, Atom Smasher
2.	September 9, 1983	Energy R&D in Biology -- Biomass
3.	September 16, 1983	Nuclear Medicine -- Parkinson's Disease -- Brookhaven
4.	September 23, 1983	Combustion and Materials Research -- Improved Fuel Burning, Tougher Materials
5.	September 30, 1983	Fusion Energy -- Basic Explanation -- TFTR
6.	October 7, 1983	Technology Transfer -- IR-100
7.	October 14, 1983	X-Rays -- Produced by Synchrotrons
8.	October 21, 1983	Small Business Innovation Research Program
9.	October 28, 1983	Carbon Dioxide and the Greenhouse Effect -- National Academy of Sciences Report
10.	November 4, 1983	Electron Microscope
11.	November 11, 1983	Gyrotron
12.	November 18, 1983	Fusion Energy -- M.I.T. Development, Alcator C
13.	November 25, 1983	Protein Mapping --ANL
14.	December 2, 1983	Supercomputers, Part 1
15.	December 9, 1983	Supercomputers, Part 2
16.	December 16, 1983	Brain Research -- PET Scanner
17.	December 23, 1983	Glassy Metals
18.	December 30, 1983	Nuclear Medicine (September 16, 1983)
19.	January 6, 1984	Combustion and Materials Research (September 23, 1983)
20.	January 13, 1984	Saturday Morning Lecture Series
21.	January 20, 1984	Superconductivity
22.	January 27, 1984	Ion Implantation for Artificial Joints

23.	February 3, 1984	Training Scientists & Engineers in science & Technology
24.	February 7, 1984	Lawrence Awards: Dr. James Jackson Dr. Michael Phelps Dr. Paul Rutherford Dr. Mark Wtighton Mr. George Zimmerman
25.	February 23, 1984	The Amazing Neutron
26.	March 3, 1984	The Amazing Neutron II

THE DEPARTMENT OF ENERGY IS ONE OF THE LARGEST SUPPORTERS OF LONG RANGE RESEARCH, MUCH OF IT AT THE VERY EDGE OF SCIENTIFIC UNDERSTANDING. MOST OF THIS IS DONE AT UNIVERSITIES AND AT THE DEPARTMENT'S NATIONAL LABORATORIES, WHICH ARE WORLD-RENOWNED AND WORLD-ENVIED. LET ME MENTION A FEW THINGS THAT DOE-SUPPORTED SCIENTISTS AND ENGINEERS ARE DOING: .

- WE DESIGN, OPERATE, AND DO RESEARCH WITH THE UNITED STATES'S MOST POWERFUL "ATOM SMASHERS". THESE HUGE MACHINES ARE USED TO PROBE NATURE'S DEEPEST SECRETS. THEY ARE LOCATED AT FERMI NATIONAL LABORATORY, STANFORD UNIVERSITY, AND BROOKHAVEN NATIONAL LABORATORY. ASIDE FROM THE SCIENTIFIC KNOWLEDGE GAINED, THE TECHNOLOGY INVOLVED IN THESE EXQUISITE CREATIONS OF BIG SCIENCE HAS LED TO MANY PRACTICAL ACCOMPLISHMENTS USED IN OUR EVERYDAY LIFE.
- DOE OPERATES THE WORLD'S LARGEST COLLECTION OF SUPERCOMPUTERS --MACHINES THAT CAN DO OVER 100 MILLION ARITHMETIC STEPS IN ONE SECOND. THE WORK DONE ON THESE MACHINES RANGES OVER NEARLY EVERY ASPECT OF MODERN SCIENCE AND ENGINEERING. FOR EXAMPLE, COMPUTERS ARE USED FOR UNDERSTANDING THE HUNDREDS OF CHEMICAL REACTIONS THAT TAKE PLACE WHEN THE GASOLINE IN YOUR CAR BURNS. SUPERCOMPUTERS ARE GOING TO BE OF GREATEST IMPORTANCE IN THE FUTURE -- INDEED, THEY ARE TODAY. THE DOE IS INVOLVED IN DEVELOPING THE NEXT GENERATION OF THESE MACHINES.
- IN THE FIELD OF NUCLEAR MEDICINE, THE TECHNIQUES OF NUCLEAR SCIENCE FOR DIAGNOSING AND TREATING OF DISEASES IS LARGELY A PRODUCT OF DOE SCIENTISTS. OVER 70 MILLION NUCLEAR MEDICINE PROCEDURES ARE DONE EVERY YEAR IN U.S. HOSPITALS. PATIENTS BENEFIT DIRECTLY FROM THIS RESEARCH.

- DURING THE COURSE OF THEIR RESEARCH ON THESE, AND HUNDREDS OF OTHER TOPICS, DOE-SPONSORED SCIENTISTS HAVE WON NOBEL PRIZES AND MANY OTHER AWARDS FOR SCIENTIFIC ACHIEVEMENT.

THE KNOWLEDGE THAT WILL COME FROM THIS PROGRAM OF RESEARCH IS ALMOST SURE TO AFFECT OUR LIVES, AND EVEN MORE SURE TO AFFECT THOSE OF OUR CHILDREN. THE STORY OF THE RESEARCH BEING DONE, AND HOW IT IS IMPORTANT TO THE UNITED STATES IN ITS COMPETITION FOR TECHNOLOGY MARKETS, WORLDWIDE, IS AN EXCITING ONE.

E.B. THE DEPARTMENT OF ENERGY HAS AN ENERGY RESEARCH BUDGET OF ABOUT $1.7 BILLION SUPPORTING RESEARCH IN SOME 60 LABORATORIES ACROSS THE NATION AND EVERYTHING FROM ADVANCED FUSION CONCEPTS TO SOLID STATE PHYSICS TO HEALTH AND ENVIRONMENTAL RESEARCH. ONE OF THE TOOLS OF THIS RESEARCH IS A PARTICLE ACCELERATOR. DR. TRIVELPIECE EXPLAINS HOW AND WHY IT'S USED.

A. T. AN ACCELERATOR IS A DEVICE THAT PERMITS A SMALL PIECE OF MATTER, AN ATOM OR SUBPART OF AN ATOM, TO BE ACCELERATED TO VERY HIGH SPEED WHERE IT CAN SERVE ITSELF AS A PROBE TO LOOK INTO STILL MORE FUNDAMENTAL PARTS OF MATTER. AS MAN'S UNDERSTANDING HAS PROGRESSED FROM SOLIDS AND LIQUIDS AND GASES DOWN TO RECOGNIZING THAT THESE ARE MADE UP OF ATOMS, CURIOSITY HAS NATURALLY OCCURRED TO BRING US TO THE QUESTION OF "WHAT ARE ATOMS MADE OF ?" WE KNOW NOW THAT ATOMS ARE MADE UP OF PROTONS AND NEUTRONS AND ELECTRONS THAT GO AROUND A COLLECTION OF PROTONS AND NEUTRONS THAT MAKE UP THE NUCLEUS OF THE ATOM. THE CURIOSITY THAT HAS CAUSED US TO LOOK AT THESE THINGS HAS REQUIRED THAT WE USE SOME UNUSUAL TOOLS, FOR EXAMPLE, TRYING TO LOOK INTO THE INTERIOR OF AN ATOM IS ROUGHLY LIKE TRYING TO IMAGINE HOW YOU WOULD FIND A FEW BILLIARD BALLS THAT WERE HIDDEN IN A LARGE BALE OF HAY. ASK YOURSELF, HOW COULD YOU FIND THE BILLIARD BALLS, WHERE THEY ARE LOCATED IN THE HAY, HOW MANY OF THEM THERE ARE, AND HOW BIG ARE THEY? ONE WAY YOU MIGHT GO ABOUT DOING THIS IS TO TAKE A RIFLE AND SHOOT THE RIFLE IN SUCH A WAY THAT THE BULLETS WOULD PASS

THROUGH THE BALE OF HAY. SOME OF THE BULLETS WOULD PASS DIRECTLY THROUGH, BUT OTHERS WOULD COME OUT AT ODD DIRECTIONS, DEPENDING ON WHETHER OR NOT THEY'VE HIT ONE OF THE BILLIARD BALLS. BY STUDYING WHERE THE BULLETS CAME OUT, YOU COULD DISCOVER WHERE, AND HOW MANY, AND HOW BIG, THE BILLIARD BALLS WERE IN THAT BALE OF HAY. IT'S ROUGHLY THE SAME PROCESS IN TRYING TO LOOK INTO THE INTERIOR OF AN ATOM. BY TAKING A VERY HIGH SPEED ELECTRON AND INJECTING IT INTO THE ATOM, AND DISCOVERING WHERE IT COMES OUT AS A RESULT OF THE FORCES THAT IT EXPERIENCES WHILE PASSING THROUGH THE ATOM, PERMITS YOU TO DETERMINE HOW BIG THE ATOM IS AND WHAT SOME OF ITS INTERNAL CHARACTERISTICS ARE.

E.B. SO THE ACCELERATOR, OR ATOM SMASHER, IS A KIND OF LOOKING GLASS THAT CAN HELP REVEAL THE MYSTERY AND SOLUTIONS TO OUR LIVES IN THE ENERGY ARENA.

E.B. THE U.S. DEPARTMENT OF ENERGY CONDUCTS BIOLOGICAL RESEARCH IN MANY AREAS, SOME OF THEM DEAL WITH BETTER WAYS TO PRODUCE ENERGY, PARTICULARLY IN THE FIELD OF BIOMASS, AND SOME OF THE RESEARCH IS DEVOTED TO THE POSSIBLE HEALTH HAZARDS OF AN ENERGY TECHNOLOGY OR RADIATION TECHNOLOGY. DR. ALVIN TRIVELPIECE IS IN CHARGE OF DOE'S ENERGY RESEARCH EFFORT, AND HE OUTLINES SOME WORK CURRENTLY BEING DONE AT A SAN FRANCISCO LABORATORY.

A.T. ONE OF THE AREAS THAT IS PARTICULARLY INTERESTING IS BEING CONDUCTED AT THE LABORATORY OF RADIOBIOLOGY AND ENVIRONMENTAL HEALTH IN SAN FRANCISCO. THIS RESEARCH INVOLVES THE USE OF MICE EMBRYOS WHICH UNDERGO CELL DIVISION FROM A SINGLE CELL TO MANY CELLS. AS THEY BEGIN THEIR DIVISION PROCESS, IT HAS BEEN DISCOVERED THAT THEY, AT FIRST, ARE TWO CELLS AND THEN FOUR CELLS. THESE CELLS CAN BE LAID ON A SINGLE PLANE. AS THEY DIVIDE AGAIN AND BECOME EIGHT, YOU NOW CANNOT PUT THEM ON TO A SINGLE PLANE ANYMORE, BUT IT HAS SOME VOLUME. WHEN THEY DIVIDE AGAIN AND BECOME SIXTEEN, SOME OF THE CELLS ARE NOW ON THE INSIDE AND SOME ARE ON THE OUTSIDE. THE FASCINATING ASPECT OF THIS RESEARCH IS THAT IT IS REVEALED THAT THOSE CELLS THAT ARE ON THE INSIDE REMAIN PERMANENTLY ON THE INSIDE, AND THEY BECOME THE MOUSE FETUS. THOSE CELLS THAT ARE ON THE OUTSIDE REMAIN PERMANENTLY ON THE OUTSIDE AND BECOME THE PLACENTA. WHAT DR. ROGER PETERSON, A SCIENTIST AT THAT

LABORATORY, HAS DISCOVERED IS THAT BY USING AN ENZYME, HORSERADISH PEROXIDASE, AND PUTTING IT INTO ONE OF THE CELLS AT ONE STAGE IN THIS CELL DIVISION PROCESS, THAT THAT CELL CAN BE STAINED AND IDENTIFIED FROM ALL THE OTHER CELLS THAT MAKE UP THE INITIAL CELL MULTIPLICATION PROCESS. THAT CELL CAN THEN BE TRACKED TO DISCOVER ITS ULTIMATE FATE AS IT THEN SUBSEQUENTLY REDIVIDES AND MAY BECOME PARTS OF THE HEART, LIVER, LUNG, SPLEEN, OR WHATEVER OF THE MOUSE. BY INTRODUCING CHEMICAL ELEMENTS INTO THE PROCESS, AT SOME STAGE, IT IS DISCOVERED THAT SOME KINDS OF DOMINANT LETHAL MUTATIONS MIGHT OCCUR IN THIS PROCESS AND GIVES US SOME IDEA OF THE POTENTIAL HAZARDS OR THE KINDS OF THINGS THAT CAN BE DONE TO AVOID THE HAZARDS ASSOCIATED WITH VARIOUS CHEMICALS ASSOCIATED WITH THE ENERGY PRODUCTION PROCESSES.

E.B. LAWRENCE BERKELEY LABORATORY SCIENTISTS HAVE IDENTIFIED FIVE GENES THAT CONTROL THE FIRST STEPS OF PHOTOSYNTHESIS. ARE THERE ANY SPINOFFS IN THE ENERGY AREA FOR THIS DISCOVERY?

A.T. PHOTOSYNTHESIS IS THE PROCESS BY WHICH SUNLIGHT, TOGETHER WITH CARBON DIOXIDE, CONVERT INTO LIVING PLANT TISSUE PLUS WATER. THIS PLANT TISSUE, OR AS WE CALL IT, BIOMASS, IS A POTENTIAL SOURCE OF ENERGY. THE PROCESS OF PHOTOSYNTHESIS ITSELF IS NOT VERY WELL UNDERSTOOD FROM A FUNDAMENTAL POINT

OF VIEW. THAT IS, WE REALLY JUST DON'T KNOW HOW SUNLIGHT MODIFIES THE MOLECULAR STRUCTURE OF PLANT MATTER IN ORDER TO CREATE NEW TISSUE AND WATER, AND POTENTIALLY THEN, ENERGY. SCIENTISTS AT SEVERAL OF OUR LABORATORIES, ARGONNE, FOR EXAMPLE, ARE ENGAGED IN STUDIES OF THE PHYSICS OF THIS PROCESS. THEY WOULD LIKE TO DETERMINE WHETHER OR NOT THERE IS A CHEMICAL OR NON-LIVING EQUIVALENT TO PHOTOSYNTHESIS SO THAT ENERGY CAN BE EXTRACTED FROM SUNLIGHT AND CONVERTED DIRECTLY INTO CHEMICAL ENERGY FOR SUBSEQUENT USE. FOR INSTANCE, IN LIVING PLANT TISSUE THE BIOMASS PRODUCT IS, AT BEST, ABOUT 2% EFFICIENT AT THE MOMENT. GENETIC ENGINEERING MIGHT MAKE IT POSSIBLE TO MAKE PLANTS MORE EFFICIENT. AS YOU INDICATED, THERE HAVE BEEN RECENTLY SOME STUDIES THAT OUR SCIENTISTS AT THE LAWRENCE BERKELEY LABORATORY HAVE DONE THAT MAKE IT APPEAR THAT THERE ARE ABOUT FIVE GENES THAT CONTROL THE PROCESS OF PHOTOSYNTHESIS. THE KIND OF BASIC RESEARCH THAT IS INVOLVED IN BOTH THIS STUDY AND THE STUDY AT ARGONNE ARE KEY TO MAKING PHOTOSYNTHESIS AN EFFICIENT PROCESS FOR ENERGY PRODUCTION.

E.B. DOE'S BIOLOGICAL RESEARCH CAN HELP IMPROVE WAYS OF PRODUCING SOME KINDS OF ENERGY AS WELL AS MORE ENERGY-EFFICIENT WAYS OF PRODUCING FOOD.

E.B. More than 40 years ago, the U.S. Department of Energy and its predecessor agencies, the Atomic Energy Commission and the Energy Research and Development Administration, has supported Health and Environmental Research Programs at national laboratories, universities, and research institutes. One area of this research is in the field of nuclear medicine. It includes techniques and instruments that aid in the diagnosis of illnesses and was instrumental in the development of the computer-assisted tomography scanner known as the CAT-scan, as well as treatments for Parkinson's disease. To learn more about this research, we talked with DOE's Director of Energy Research, Dr. Alvin Trivelpiece.

A.T. The origins of this research program are very interesting. They date back to 1946, when Congress created the Atomic Energy Commission. The Congress directed the Atomic Energy Commission to do several things and this includes making contracts, agreements, grants and aids, and loans, for the utilization of fissionable and radioactive materials for medical and health purposes, and for the protection of health during research and production activities involving nuclear materials. As the Atomic Energy Commission went into the Energy Research and Development Administration and new responsibilities were added to the activities, it was then assigned the responsibility of engaging in and supporting environmental, physical, and

SAFETY RESEARCH RELATED TO THE DEVELOPMENT OF ENERGY SOURCES AND UTILIZATION TECHNOLOGIES. PART OF THAT RESPONSIBILITY THEN INCLUDED WHAT HAS BECOME KNOWN AS THE FIELD OF NUCLEAR MEDICINE. ITS OBJECTIVE IS TO DEVELOP THE HIGHEST POTENTIAL APPLICATION OF NUCLEAR SCIENCE TO THE DIAGNOSIS AND TREATMENT OF HUMAN DISEASE. THESE TECHNIQUES INCLUDE THINGS THAT INVOLVED DIAGNOSIS FOR HEART DISEASE AND FOR DIAGNOSTIC SCANNING, AND SUCH THINGS AS HODGKIN'S DISEASE. ALSO, THERE ARE INSTRUMENTS THAT AID IN THE DIAGNOSIS OF VARIOUS DISEASES, AND THESE INCLUDE THINGS CALLED THE SCINTILLATION CAMERA AND SCANNING INSTRUMENTS THAT ARE NOW FAMILIAR TO THE PUBLIC. IN THE AREA OF TREATMENT, THERE ARE TWO ACTIVITIES WHICH HAVE THERE ORIGINS IN DEPARTMENT OF ENERGY PROGRAMS, AND THESE INVOLVE TREATMENT OF HYPERTHYROIDISM AND PARKINSON'S DISEASE. I'D LIKE TO CONCENTRATE JUST FOR A MOMENT ON PARKINSON'S DISEASE TO DISCUSS WHAT ITS EFFECTS ARE AND WHAT THE ROLE WAS PLAYED BY THE AEC, AND NOW THE DEPARTMENT OF ENERGY. AS YOU KNOW, PARKINSON'S DISEASE IS A DEBILITATING NEUROLOGICAL DISEASE THAT AFFLICTS CLOSE TO A MILLION PEOPLE WITH 50,000 NEW CASES EACH YEAR. IN TWO THIRDS OF THE CASES, THE ONSET OF THE SYMPTOMS OCCUR BETWEEN THE AGES OF 50 AND 70 AND BECOMES PROGRESSIVELY WORSE.

In the early 1950's, several radioisotopes, particularly manganese-56, were used to investigate a possible link between trace metals and this disease. Although no conclusive connection could be made between the disease and manganese poisoning, several new areas of research evolved from these studies. Eventually, it was found that there is a deficiency of an amino acid, dopamine, in the brains of persons suffering from Parkinson's disease and that this amino acid could be synthesized internally after the intravenous injection of a related compound called L-dopa. The treatment does not cure the disease, but can mitigate the severity of its progression. It produces initial improvement in 50% to 75% of the cases, slows the rate of advance of the disease and decreases the mortality rate. Thus the benefits of this treatment can be measured in terms of improved quality of life with an average increase of about 2.5 person-years of active productive time per person afflicted. Based on about 50,000 new cases per year in the United States, this translates to a gain of approximately 125,000 person-years of active life annually. This kind of nuclear medicine development by the Department of Energy is not one of the things which the Department is normally known to be involved in, but has been an important activity through

THE YEARS STARTING WITH THE ATOMIC ENERGY COMMISSION, BEING CONTINUED WITH THE ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION, AND NOW BEING SUPPORTED BY THE DEPARTMENT OF ENERGY.

E.B. BROOKHAVEN NATIONAL LABORATORY, ON LONG ISLAND, NEW YORK, WAS A KEY CONTRIBUTOR TO THE PARKINSON'S DISEASE RESEARCH EFFORT. DOE'S RESEARCH PROGRAM WILL CONTINUE TO LEAD IN MAKING FUNDAMENTAL AND PRACTICAL CONTRIBUTIONS IN REDUCING UNCERTAINTIES ON HEALTH AND ENVIRONMENTAL ASPECTS OF THE MERGING ENERGY TECHNOLOGIES.

E.B. MOST OF THE ENERGY RESOURCES USED IN THE UNITED STATES ARE BURNED TO RELEASE THEIR ENERGY. HOWEVER, NOT ALL OF THE COMBUSTION PROCESS IS COMPLETELY UNDERSTOOD, RESULTING IN A LOSS OF POTENTIAL ENERGY USE AND POLLUTION. FOR EXAMPLE, A CAR ENGINE GETS ONLY ABOUT 30% OF THE POTENTIAL ENERGY OUT OF THE FUEL IT BURNS. COMBUSTION RESEARCH, CONDUCTED BY THE ENERGY DEPARTMENT, IS AIMED AT IMPROVING NOT ONLY COMBUSTION EFFICIENCY, BUT ALSO IN REDUCING POLLUTION, AS THE DIRECTOR OF THE DEPARTMENT OF ENERGY'S OFFICE OF ENERGY RESEARCH, DR. ALVIN TRIVELPIECE, EXPLAINS.

A.T. IT'S RATHER IRONIC THAT EVEN THOUGH FIRE IS ONE OF MAN'S OLDEST INVENTIONS, THE PROCESSES THAT ARE INVOLVED IN BURNING, OR COMBUSTION, ARE VERY POORLY UNDERSTOOD. THE REASON HAS TO DO WITH THE COMPLEXITY OF THE VARIOUS PROCESSES THAT ARE INVOLVED. THERE ARE, LITERALLY, DOZENS OF CHEMICAL REACTIONS THAT ARE ALL OCCURRING SIMULTANEOUSLY, AND IN ADDITION, THIS PROCESS OF BURNING LEADS TO A VERY VIOLENT STIRRING DUE TO THE ENERGY RELEASE, AND THIS IS CALLED TURBULENCE. TO SOME EXTENT, IT IS HARDER TO UNDERSTAND THE SIMPLE PROCESSES IN A FLAME THAN IT IS THOSE IN A NUCLEAR REACTOR.

WHY SHOULD WE WANT TO UNDERSTAND COMBUSTION? MOST OF OUR USE OF ENERGY IS THROUGH COMBUSTION, CARS, HOUSEHOLD HEATING, COOKING, AND POWER GENERATION. THERE IS THE POSSIBILITY TO IMPROVE EFFICIENCY AND REDUCE POLLUTION IF WE UNDERSTOOD IT BETTER. TWO RECENT DEVELOPMENTS GIVE US HOPE OF FAR BETTER UNDERSTANDING. IT TURNS OUT THAT LASER BEAMS CAN BE USED AS A TOOL TO EXAMINE FLAMES AND VERY FAST COMPUTERS THAT ARE NEEDED TO CALCULATE THE CHEMICAL REACTIONS ARE NOW AVAILABLE. WITH THE LASER, WE CAN LOOK AT A VERY TINY POINT INSIDE A FLAME AND MEASURE THE TEMPERATURE AND THE DENSITY OF THE FLAME AS IT'S GOING, SAY INSIDE THE CYLINDER OF RUNNING INTERNAL COMBUSTION ENGINE AT ONE MILLIONTH OF A SECOND INTERVALS. WE CAN MEASURE THE TEMPERATURE, THE CONCENTRATION OF ALL THE MOLECULES, AND HOW THE BURNING GASES ARE MOVING. IT MAY BE POSSIBLE IN THE NOT TO DISTANT FUTURE TO USE THIS RESEARCH TO DESIGN BETTER CAR ENGINES. DOE SCIENTISTS WORK WITH INDUSTRY SCIENTISTS AND ENGINEERS AT THE COMBUSTION RESEARCH FACILITY, WHICH IS LOCATED AT THE SANDIA LABORATORY IN LIVERMORE, CALIFORNIA.

E.B. DR. TRIVELPIECE ALSO NOTES THAT DOE IS CONDUCTING MATERIALS RESEARCH TO IMPROVE ENERGY EFFICIENCY AND REDUCE DEPENDENTS ON IMPORTED STRATEGIC MINERALS.

A.T. IT WOULD TAKE A LONG TIME TO GO INTO DETAIL IN ALL THE VARIOUS AREAS IN WHICH THE DEPARTMENT OF ENERGY SUPPORTS ADVANCED MATERIALS RESEARCH. HOWEVER, ONE, FROM AN ENERGY POINT OF VIEW, THAT IS PARTICULARLY INTERESTING INVOLVES HIGH TEMPERATURE MATERIALS. AS YOU KNOW, MANY ASPECTS OF MODERN LIVING DEPENDS ON HIGH TEMPERATURE MATERIALS: JET ENGINES, MANUFACTURING PROCESSES, AND POWER GENERATION, FOR EXAMPLE.

USUALLY PROCESSES THAT USE OR PRODUCE ENERGY ARE MORE EFFICIENT AT HIGHER TEMPERATURES. SUITABLE MATERIALS MUST REMAIN STRONG WHEN THEY ARE HOT AND ALSO MUST NOT OXIDIZE, OR BURN UP, AS THEY ARE USED. AT VERY HIGH TEMPERATURES, STEEL ISN'T A GOOD MATERIAL. MOST HIGH TEMPERATURE MATERIALS ARE ALLOYS CONTAINING THE METALS CHROMIUM, COBALT, AND NICKEL. THESE METALS ARE EXPENSIVE, AND ALSO, IN THE CASE OF CHROMIUM AND COBALT, ARE IMPORTED FROM OVERSEAS. RECENT DOE RESEARCH HAS LED TO THE DEVELOPMENT OF VERY PROMISING HIGH TEMPERATURE MATERIALS THAT CONTAIN NO CHROMIUM OR COBALT. THESE MATERIALS ARE CALLED INTERMETALLICS, AS THEY INVOLVE THE COMPOUND OF TWO METALS RATHER THAN SOLUTIONS. IN THIS CASE, NICKEL AND ALUMINUM IS A COMPOUND THAT IS CALLED NICKEL ALUMINIDE. IN THE PAST, SUCH COMPOUNDS HAVE BEEN BRITTLE, WHICH BASICALLY RULED OUT THEIR USE. BY ADDING TINY AMOUNTS

OF THE ELEMENT BORON TO THE NICKEL ALUMINIDE, DOE SCIENTISTS HAVE OBTAINED A VERY HIGH TEMPERATURE MATERIAL THAT SHOWS GREAT PROMISE. IT IS STRONG AT HIGH TEMPERATURES, IT REMAINS DUCTILE, RATHER THAN BEING BRITTLE, IT IS VERY RESISTANT TO OXIDIZATION, AND IT CONTAINS NO CHROMIUM OR COBALT. SEVERAL INDUSTRIES ARE VERY INTERESTED IN THIS DEVELOPMENT BY THE DEPARTMENT. MOST OF THIS WORK IS BEING DONE AT THE OAK RIDGE NATIONAL LABORATORY IN OAK RIDGE, TENNESSEE.

E.B. ENERGY EFFECTS ALMOST EVERY ASPECT OF OUR LIVES, AND DOE SCIENTISTS ARE CONTINUALLY WORKING ON BETTER WAYS TO USE AND PRODUCE THIS VERY VITAL COMMODITY.

E.B. OUR SUN IS A GIGANTIC FUSION REACTOR, AND FOR MANY YEARS, SCIENTISTS HAVE BEEN TRYING TO DUPLICATE THE SUN, ON A SMALL SCALE, TO PROVIDE AN ALMOST LIMITLESS ENERGY SOURCE FOR OUR PLANET BECAUSE THE FUEL COULD BE DERIVED FROM WATER. BUT, COPYING MOTHER NATURE IS NOT EASY AS WE LEARN FROM THE DIRECTOR OF ENERGY RESEARCH AT THE UNITED STATES DEPARTMENT OF ENERGY, DR. ALVIN TRIVELPIECE.

A.T. FUSION, IN THE ENERGY CONTEXT, MEANS THE FUSION OR JOINING OF TWO NUCLEI OF SOME ISOTOPES OF HYDROGEN, WHICH IS OUR LIGHTEST AND MOST ABUNDANT ELEMENT. THESE TWO ISOTOPES, CALLED DEUTERIUM AND TRITIUM, ARE LIKE HYDROGEN IN THAT THEY EACH HAVE ONE PROTON IN THEIR NUCLEUS, BUT, IN ADDITION, THEY ALSO HAVE RESPECTIVELY, ONE AND TWO NEUTRONS IN THEIR NUCLEUS. THESE NEUTRONS GIVE RISE TO THE NUCLEAR PROPERTY THAT OCCURS WHEN A DEUTERIUM AND TRITIUM NUCLEUS ARE SLAMMED TOGETHER AT HIGH ENOUGH SPEED TO OVERCOME THEIR MUTUAL REPULSION DUE TO BOTH BEING POSITIVELY CHARGED OBJECTS. THAT IS, THEY FUSE TOGETHER AND CREATE A DIFFERENT ELEMENT, HELIUM, AND ALSO RELEASE SOME ENERGY WHICH APPEARS IN THE FORM OF A NEUTRON MOVING AT HIGH SPEED. THE SOURCE OF THIS ENERGY COMES FROM THE FACT THAT THE PRODUCTS, AFTER FUSION, HAVE LESS MASS. THIS CHANGE OF MASS HAS BEEN CONVERTED TO ENERGY ACCORDING TO EINSTEIN'S FAMOUS FORMULA, $E=MC^2$. ALTHOUGH THE AMOUNT OF ENERGY RELEASED IN THIS

SINGLE FUSION EVENT IS REALLY QUITE SMALL, THE CUMULATIVE EFFECT OF MANY SUCH SIMILAR FUSION EVENTS IS WHAT KEEPS THE SUN BURNING AND IS THE BASIS FOR THE DESTRUCTIVE POWER OF THERMONUCLEAR WEAPONS. IT IS OUR HOPE AND EXPECTATION THAT THIS THERMONUCLEAR PROCESS CAN BE CONTROLLED TO RELEASE ENERGY IN SUCH A WAY AS TO GENERATE ELECTRICITY OR SERVE AS A HEAT SOURCE FOR SOME OTHER PROCESS. THIS RESEARCH TO DEVELOP THIS OPTION WAS INITIATED IN SEVERAL COUNTRIES IN ABOUT 1952 CN A CLASSIFIED BAS'S. IN 1958, THE RESEARCH WAS DECLASSIFIED. TODAY, THERE IS SUBSTANTIAL INTERNATIONAL COOPERATION IN THIS IMPORTANT FIELD OF RESEARCH. ONE OF THE REASONS WHY THERE IS SUCH INTENSE INTEREST IN FUSION STEMS FROM THE FACT THAT THE FUEL IS, FOR ALL PRACTICLE PURPOSES, INEXHAUSTIBLE. EVEN THOUGH ONLY ABOUT ONE IN EVERY 6,500 MOLECULES OF WATER CONTAINS THE DEUTERIUM ATOM, THERE IS A LOT OF WATER ON EARTH. THIS FUSION FUEL IS EASILY EXTRACTED FROM WATER. TO GIVE YOU SOME IDEA OF THE ENERGY CONTENT, IMAGINE THAT WE HAD ONE CUBIC CENTIMETER OF WATER WHERE EACH MOLECULE HAS A DEUTERIUM ATOM IN IT. THIS CUBIC CENTIMETER OF SO CALLED "HEAVY WATER" HAS THE ENERGY CONTENT OF 300 GALLONS OF GASOLINE. IT TURNS OUT THAT IN ORDER TO IGNITE THIS FUSION BURNING PROCESS, IT IS NECESSARY TO CREATE AND CONTAIN A GAS MIXTURE OF

DEUTERIUM AND TRITIUM AT TEMPERATURES GREATER THAN THOSE OF OUR SUN; OVER 100 MILLION DEGREES. THIS IS NOT EASY BECAUSE SUCH HOT GASES MUST NOT TOUCH ANY SOLID OBJECTS.

SCIENTISTS HAVE DEVISED SEVERAL WAYS TO HOLD ONTO THESE HOT GASES WHICH ARE CALLED PLASMAS. ONE OF THESE INVOLVES THE USE OF MAGNET COILS ARRANGED IN A CIRCLE SO AS TO CREATE A REGION INSIDE WITH A SHAPE OF A DONUT. THESE DONUT SHAPED MAGNETIC FIELDS ARE USED TO CREATE, HEAT, AND STUDY THE PROPERTIES OF THESE HOT PLASMAS. THERE HAS BEEN STEADY PROGRESS OVER NEARLY 30 YEARS OF INTENSE RESEARCH IN THIS FIELD. THE DEPARTMENT OF ENERGY RECENTLY COMMISSIONED INITIAL OPERATION OF A $314 MILLION EXPERIMENT AT ITS PRINCETON PLASMA PHYSICS LABORATORY CALLED THE TFTR FOR TOKAMAK FUSION TEST REACTOR. THIS DEVICE WILL BE READY TO CONDUCT EXPERIMENTS THAT DEMONSTRATE THIS FUSION BURNING PROCESS IN ABOUT 1985. BEYOND THIS INITIAL DEMONSTRATION, CONSIDERABLE WORK WILL BE REQUIRED TO HARNESS FUSION INTO A PRACTICLE ENERGY DELIVERY SYSTEM. THIS IS ONE OF THE REASONS WHY IT IS DIFFICULT TO PREDICT EXACTLY WHEN THIS INEXHAUSTIBLE ENERGY RESOURCE MIGHT BE AVAILABLE. EXPERIENCE WITH OTHER ENERGY GENERATING TECHNOLOGIES SUGGESTS THAT IT IS NOT LIKELY TO BE LESS THAN 20 YEARS BEFORE WE MIGHT HAVE OUR FIRST FUSION POWER

PLANT. THIS WILL NO DOUBT DEPEND ON THE RATE OF PROGRESS OUR SCIENTISTS AND ENGINEERS ACHIEVE, AS WELL AS GENERAL ECONOMIC AND ENERGY SUPPLY CONSIDERATIONS. THE U.S. IS AMONG THE LEADERS IN THIS FIELD WHICH ALSO IS ACTIVELY PURSUED IN THE EUROPEAN COMMUNITIES, JAPAN, AND THE SOVIET UNION.

FUSION ENERGY HAS MANY DESIRABLE FEATURES AND THERE IS EVERY REASON TO BELIEVE THAT IT CAN BE MADE TO WORK EVENTUALLY AND TAKE ITS PLACE AS ONE OF OUR MAJOR ENERGY RESOURCES.

E.B. SOMEDAY THE ENERGY SOURCE OF THE STARS COULD PROVIDE ENERGY FOR OUR HOMES AND BUSINESSES.

E.B. Many of the Nation's greatest inventions have been made by individuals, or small companies, working on tight budgets. The inventions, or discoveries, often had immediate application and payoff. As the scope of science expanded and the cost of carrying on research increased, with economic benefits of the research extending years out into the future, many people and businesses were excluded from some scientific research projects. Sometimes the cost of a single scientific instrument can range from hundreds of thousands to millions of dollars. In these high-risk, long-term payoff research projects, the Federal Government, working with universities and private businesses, pool their resources to search for answers to our 20th century, and, soon to be our 21st century problems. When the answers are found, the technology is transferred to the private sector, so the public can benefit from the research they help fund. The Energy Department has several laboratories dedicated to these high-risk research projects, and their research efforts are often award winning as the Director of DOE's Office of Energy Research, Dr. Alvin Trivelpiece, explains.

A.T. The Department of Energy supports programs of basic and applied research in many areas. This research leads to important discoveries and inventions. Many of these inventions find their way out of DOE's laboratories and into commercial application, particularly in the high technology area.

EACH YEAR INDUSTRIAL RESEARCH AND DEVELOPMENT MAGAZINE HAS A COMPETITION TO DETERMINE THE 100 BEST TECHNOLOGY ACHIEVEMENTS BY RESEARCH ORGANIZATIONS IN THE UNITED STATES. AMONG THE 1983 IR-100 WINNERS WERE 14 WINNERS FROM DOE LABORATORIES. THESE INCLUDE: FROM THE ARGONNE NATIONAL LABORATORY A TWO-DIMENSIONAL POSITION SENSITIVE NEUTRON SCINTILLATION DETECTOR. FROM OAK RIDGE NATIONAL LABORATORY THERE WERE SIX WINNERS, ONE OF WHICH IS FOR AN INTERMETALLIC ALLOY CALLED NICKEL ALUMINIDE. FERMI NATIONAL LABORATORY HAD, AMONG ITS FIVE WINNERS, A PRECISION ELECTRIC CURRENT SENSOR. LOS ALAMOS NATIONAL LABORATORY WAS THE RECIPIENT OF AN AWARD FOR A TRANSURANIC WASTE ASSAY SYSTEM. THE LAWRENCE LIVERMORE NATIONAL LABORATORY FOR AN ELECTRONIC MICRODRYER, AND PACIFIC NORTHWEST LABORATORY WON AN AWARD FOR A SUPERCRITICAL FLUID CHROMATOGRAPH/MASS SPECTROMETER.

ONE OF THE WINNERS FROM OAK RIDGE NATIONAL LABORATORY (ORNL) IS OF PARTICULAR INTEREST. THIS INTERMETALLIC ALLOY (NICKEL ALUMINIDE) HAS HIGH TEMPERATURE STRENGTH AND CORROSION RESISTANCE SUPERIOR TO THE HIGHEST STAINLESS STEEL AND SUPERALLOYS. THIS NICKEL-IRON "ALUMINIDE" IS ONE OF A NEW CLASS OF LIGHTWEIGHT STRUCTURAL ALLOYS MADE OF ABUNDANT LOW-COST MATERIALS.

THESE INTERMETALLIC COMPOUNDS, SUCH AS THE ALUMINIDES, SHARE CHARACTERISTICS OF BOTH METALS AND CERAMICS. INHERENTLY, THEY ARE VERY STRONG AND CORROSION- AND HIGH TEMPERATURE-RESISTANT. UNTIL NOW THEY ALSO HAVE BEEN EXTREMELY BRITTLE; A QUALITY THAT GREATLY LIMITED THEIR USE AS STRUCTURAL MATERIALS.

THIS NEW ALLOY IS EASY TO USE. IT IS MADE OF LIGHTWEIGHT AND INEXPENSIVE MATERIALS, SUCH AS ALUMINUM, AND IS THREE TO SIX TIMES STRONGER THAN TODAY'S BEST STAINLESS STEELS AT HIGH TEMPERATURES. THIS ALLOY WAS DEVELOPED IN OAK RIDGE NATIONAL LABORATORY'S METALS AND CERAMICS DIVISION.

AT ROOM TEMPERATURE, THE MATERIAL'S STRENGTH IS COMPARABLE TO COMMERCIAL SUPERALLOYS, BUT ACTUALLY BECOMES STRONGER AT HIGHER TEMPERATURES. IT CAN WITHSTAND TEMPERATURES AS HIGH AS 1000 DEGREES C (1830 DEGREES F), COMPARED TO 600 DEGREES C FOR CHROMIUM-BASED STEELS AND 800 DEGREES C FOR DUCTILE SUPERALLOYS.

ALTHOUGH THIS COMPETITION INVOLVES ONLY A LIMITED AREA OF HIGH TECHNOLOGY, IT ILLUSTRATES SOME OF THE ACTIVITIES IN WHICH DOE RESEARCH LEADS TO TECHNOLOGY TRANSFER OF BENEFIT TO THE NATION.

IN THE 19 YEARS SINCE THE AWARDS HAVE BEEN MADE, OAK RIDGE NATIONAL LABORATORY HAS RECEIVED A TOTAL OF 32 AWARDS, AND ARGONNE NATIONAL LABORATORY HAS RECEIVED A TOTAL OF 23 AWARDS.

E.B. ALTHOUGH DOE LABORATORIES ARE PRIMARILY ENERGY RESEARCH ORIENTED, THEIR EFFORTS OFTEN CROSS MANY BOUNDARIES. IN THE ENERGY AREA, THE LABORATORIES ARE WORKING ON IMPROVING ENERGY CONSERVATION TECHNOLOGIES; RENEWABLE ENERGY RESOURCES, SUCH AS SOLAR; MAGNETIC FUSION, WHICH COULD BE OUR PRINCIPAL ENERGY SOURCE IN THE FUTURE; IMPROVING FOSSIL FUEL TECHNOLOGIES; AND IN MANY AREAS OF NUCLEAR ENERGY.

LET ME BRIEFLY DESCRIBE THE USE OF SYNCHROTRON RADIATION IN ONE MEDICAL APPLICATION. THERE ARE ABOUT ONE MILLION HEART ATTACKS IN THE UNITED STATES EACH YEAR. HALF OF THESE ARE FATAL AND OF THESE, HALF ARE SUDDEN DEATHS OF PERSONS THOUGHT TO BE IN GOOD HEALTH. PREVENTING DISEASE OF THE CORONARY ARTERIES IS OUR LEADING HEALTH PROBLEM. IF DIAGNOSED EARLY, THEY CAN BE TREATED WITH DRUGS OR WITH CORONARY BYPASS SURGERY. CONVENTIONAL METHODS OF DIAGNOSIS LEAVE MUCH TO BE DESIRED. WHAT IS NEEDED IS A MEANS OF OBTAINING A CLEAR X-RAY PICTURE OF A BEATING HEART AND PULSING ARTERIES. A SYNCHROTRON LIGHT SOURCE IS CAPABLE OF PRODUCING X-RAYS THAT HAVE THE RIGHT COLOR, BRIGHTNESS, AND PULSE LENGTH TO PERMIT STOP-ACTION X-RADIOGRAPHY, AND TO FREEZE THE MOTION OF CORONARY ARTERIES.

THE USE OF X-RAYS HAS NOT ONLY BECOME QUITE COMMON IN MEDICAL DIAGNOSIS BUT ALSO IN COUNTLESS INDUSTRIAL APPLICATIONS. THIS HIGHLY PENETRATING SHORT WAVELENGTH RADIATION IS USUALLY PRODUCED BY CREATING SOME HIGH SPEED ELECTRONS SIMILAR TO ELECTRON BEAMS THAT MAKE TV PICTURES. THESE HIGH SPEED ELECTRONS ARE ABRUPTLY BROUGHT TO REST AS THEY ARE DRIVEN INTO A METAL TARGET. IT IS THIS PROCESS OF RAPID DECELERATION THAT CREATES X-RAYS. ALTHOUGH X-RAYS CAN'T BE SEEN, IT IS CONVENIENT TO USE THE ANALOGY WITH VISIBLE LIGHT AND TALK ABOUT THEIR "COLOR" AND "BRIGHTNESS". THEIR COLOR, OR MORE PROPERLY, THEIR WAVELENGTH, IS DETERMINED BY THE ELECTRONS' SPEED BEFORE THEY STRIKE THE TARGET. THE BRIGHTNESS OR INTENSITY IS DETERMINED BY THE NUMBER OF ELECTRONS THAT STRIKE THE TARGET. THE X-RAYS PRODUCED BY THESE COLLISIONS USUALLY WILL BE DIFFERENT "COLORS" AND WILL BE SPREAD OUT IN A DIFFUSE BEAM. THIS CONTRASTS WITH LASERS WHICH PRODUCE SINGLE COLOR, SHARPLY FOCUSED BEAMS. IN THE LAST FEW YEARS, A NEW METHOD OF PRODUCING X-RAY BEAMS HAS BEEN DEVELOPED WHICH PRODUCES A VERY INTENSE, SHARPLY FOCUSED LASER-LIKE BEAM OF X-RAYS THAT IS THE EQUIVALENT OF ONE COLOR.

THE NEW METHOD IS BASED ON THE FACT THAT ELECTRONS ALSO EMIT X-RAYS IF THEY ARE MADE TO TURN A SHARP CORNER OR ARE GUIDED BY MAGNETS TO GO AROUND IN A CIRCLE, CAUSING THEM TO EMIT X-RAYS CONTINUOUSLY. THE COLOR OF THE EMITTED X-RAYS DEPENDS ON HOW BIG THE CIRCLE IS AND HOW FAST THE ELECTRONS ARE GOING. THE DEVICE THAT DOES THIS IS CALLED A SYNCHROTRON LIGHT SOURCE, NAMED AFTER THE TYPE OF PARTICLE ACCELERATOR IN WHICH THIS RADIATION WAS FIRST OBSERVED. AT FIRST, THIS RADIATION WAS A GREAT NUISANCE TO THE PHYSICISTS USING ACCELERATORS BECAUSE IT MEANT THAT THE ELECTRONS IN IT WERE LOSING ENERGY AND SLOWING DOWN. BUT AS IT SOMETIMES TURNS OUT, ONE PERSON'S LOSS IS ANOTHER PERSON'S GAIN. RATHER THAN LOOKING FOR WAYS TO ELIMINATE

THIS SYNCHROTRON RADIATION, SOME PHYSICISTS BEGAN LOOKING FOR WAYS TO ENHANCE IT AND USE IT IN RESEARCH APPLICATIONS. AS A RESULT, SCIENCE NOW HAS A POWERFUL NEW TOOL TO STUDY MATERIALS, BASIC RESEARCH IN BIOLOGY, AND TO MAKE MEDICAL DIAGNOSIS.

PILOT STUDIES USING THIS ADVANCED DIAGNOSTIC PROCESS ON HUMAN SUBJECTS WILL BE DONE USING THE NATIONAL SYNCHROTRON LIGHT SOURCE AT THE DEPARTMENT OF ENERGY'S BROOKHAVEN NATIONAL LABORATORY. THIS IS A COLLABORATIVE EFFORT INVOLVING SCIENTISTS FROM STANFORD UNIVERSITY, THE DEPARTMENT'S LAWRENCE BERKELEY LABORATORY, AND THE NATIONAL INSTITUTES OF HEALTH. THIS IMPORTANT USE OF SYNCHROTRON LIGHT SOURCE X-RAYS HAS THE PROSPECT OF BEING DEVELOPED INTO A SAFE, COST-EFFECTIVE, NONSURGICAL METHOD FOR DIAGNOSIS THAT COULD BE AVAILABLE AT MANY MEDICAL CENTERS IN THE FUTURE AND IS ONE OF THE MANY AREAS IN WHICH THE DEPARTMENT OF ENERGY'S SCIENTIFIC EFFORTS IN THE ENERGY AREA LEAD TO MEDICAL TOOLS THAT BENEFIT EVERYONE.

One of the problems that concerns the Department of Energy is the management of nuclear wastes. The Viking Energy Corporation, of Pittsburgh, Pennsylvania, will investigate the potential for the use of robots in the management of radioactive wastes at a Nuclear Waste Facility. Phases of construction and decommissioning will be identified which are amenable to robotic devices with a consequent increase in safety by reduction of radiological impacts. This is one of the contracts that DOE recently awarded to a small business firm. These contracts are part of a program started in DOE this year to take advantage of the skills in the small business community.

The program called the Small Business Innovation Research Program, or SBIR, is a congressionally mandated program of innovative research and development to be performed by small business firms. In the case of the Department of Energy (DOE) the SBIR budget in Fiscal Year 1983, the program's first year of implementation, was just over 5 million dollars. This amount will triple in Fiscal Year 1984.

DOE was the first agency to issue its solicitation for proposals. The solicitation covered 25 technical topics reflecting a broad spectrum of the Department's programs. The response was overwhelming. About 1,700 proposals were received. Of these, 106 were selected for funding. These

INCLUDE: A PROJECT PROPOSED BY BEND RESEARCH, INC., OF BEND OREGON. THIS PROJECT WILL SEEK TO REMOVE THE ACID GASSES, HYDROGEN SULFIDE, AND CARBON DIOXIDE FROM COAL GASES BY DEVELOPING A THIN FILM WHICH HAS A HIGH CONCENTRATION OF AN ACID-ABSORBING SOLVENT. THIS NOVEL TECHNIQUE WILL PREVENT SULFUR POLLUTION, INCREASE THE HEATING VALUE OF COAL GAS, AND REDUCE THE COST OF PRODUCING GASEOUS FUEL FROM COAL. THE SPIRE CORPORATION, OF BEDFORD, MASSACHUSETTS, PROPOSES TO DEVELOP A HIGH-EFFICIENCY, LOW-COST, FLAT-PLATE SOLAR PHOTOVOLTAIC CELL. FABRICATION OF THIS TYPE OF CELL COULD HELP TO ESTABLISH VIABLE, COST-EFFECTIVE SOLAR ELECTRICITY. THE MAXWELL LABORATORIES, OF SAN DIEGO, CALIFORNIA, PROPOSES TO DESIGN AND BUILD AN INSTRUMENT TO MEASURE AND STUDY THE AMOUNTS OF UNDESIRED IMPURITIES IN FUSION FUEL. INFORMATION FROM EXPERIMENTS WITH THIS DEVICE WILL ENABLE RESEARCHERS TO REDUCE THE LEVEL OF IMPURITIES IN ORDER TO ACHIEVE THE GOAL OF OBTAINING LARGE AMOUNTS OF SAFE, CLEAN ENERGY FROM MAGNETIC FUSION. THE MISSION RESEARCH CORPORATION, OF ALBUQUERQUE, NEW MEXICO, WILL EXPLORE THE FEASIBILITY OF A NEW CONCEPT FOR THE DESIGN OF HIGH-ENERGY PARTICLE ACCELERATORS. THIS CONCEPT USES HIGH ELECTRIC FIELDS IN AN INTENSE LASER BEAM AND COULD SIGNIFICANTLY REDUCE THE COST OF DESIGN AND CONSTRUCTION OF ACCELERATORS USED IN THE STUDY OF THE FUNDAMENTAL CONSTITUENTS OF MATTER.

THESE SBIR CONTRACTS HELP THE DEPARTMENT BY BRINGING NOVEL SOLUTIONS TO OUR ATTENTION OF MANY OF THE PROBLEMS THAT WE HAVE, AND AT THE SAME TIME, AID SMALL HIGH TECH BUSINESSES IN GETTING STARTED IN SOME PROMISING AREAS OF RESEARCH AND DEVELOPMENT IMPORTANT TO OUR NATION.

Is the earth getting warmer? Probably! Is there any immediate risk? No! Why has there been so much attention to this subject recently? I'm not sure that it deserves as much attention as it has received. The main reason for this sudden attention is that two reports were issued recently on the effect of carbon dioxide, or CO_2, on the average temperature of the earth. That's not to say that the CO_2 problem isn't important. It is! It's just that it is not urgent.

What is the problem?

Carbon dioxide, or CO_2, is a colorless, odorless, and non-poisonous gas. It is the inevitable product of combustion, that is the burning of wood, oil, gas, or coal. CO_2 is also a product of "natural" oxidation, such as occurs in the rotting of plant material. CO_2 is also the "food" of plants. Carbon is, afterall, the basis of life, both plant and animal.

Although there has always been CO_2 in the atmosphere, the amount has increased steadily since the industrial revolution,this is both from increased burning of fossil fuels and from widespread deforestation. The growth has been from about 318 parts per million (ppm) to about 348 ppm in the last 25 years. CO_2 is a so called "greenhouse" gas, that is it behaves like the glass in a greenhouse. Sunlight passes through it freely and heats the earth.

THE EARTH, IN TURN, RERADIATES ENERGY , BUT IT RERADIATES THIS ENERGY AT A LONGER WAVELENGTH. THE LONGER WAVELENGTH RADIATION IS TRAPPED. THEREFORE, THE RESULT OF INCREASED CO_2 SHOULD BE A WARMING OF THE EARTH.

THE ACTUAL PICTURE IS MUCH MORE COMPLEX. WE REALLY CAN'T PREDICT JUST HOW MUCH THE EARTH WILL WARM UP, OR HOW THIS WILL AFFECT THE CLIMATE, THAT IS THE TEMPERATURE AND THE PRECIPITATION. THERE IS GENERAL AGREEMENT THAT CONTINUING INCREASE IN CO_2 WILL CAUSE SLIGHT INCREASES IN AVERAGE TEMPERATURE, MIGHT CAUSE THE SEA LEVEL TO RISE SLIGHTLY, AND WILL MAKE PLANTS GROW FASTER AND USE LESS WATER. ALL THIS TAKES PLACE VERY SLOWLY.

DOE IS THE LEAD AGENCY IN THE GOVERNMENT-WIDE EFFORT TO UNDERSTAND ALL ASPECTS OF THE CO_2 SITUATION. THE TOTAL GOVERNMENT BUDGET FOR CO_2 RESEARCH IS ABOUT $20 MILLION PER YEAR; DOE SPENDS ABOUT $12 MILLION.

THERE WERE TWO WIDELY DISCUSSED EVENTS RELATED TO CO_2 IN MID OCTOBER. THESE ARE A REPORT SUBMITTED BY THE ENVIRONMENTAL PROTECTION AGENCY AND A REPORT PREPARED BY THE NATIONAL ACADEMY OF SCIENCES. THE CONCLUSIONS REACHED BY BOTH WERE VERY SIMILAR.

- Some warming is likely to take place.
- The sea level could rise.
- There is no realistic way of solving the problem by reducing the amount of CO_2 emitted, and most important,
- Much more research is needed.

The tone of the two reports was clearly different, at least as interpreted by much of the press.

- The EPA report sounded as if a crisis was imminent.
- The National Academy of Sciences reported that society could cope with the predicted changes with relative ease. This is because any changes that would occur would be gradual.

The National Academy of Sciences report, based largely on DOE data, concluded that warm-up is not an urgent problem. Further, much more research needs to be done before predictions can be given any credence. In any event, there is ample time to adjust to these possible changes.

Atoms are much too small to be seen by the naked eye or even with the best optical microscope. Visible light lets us see billions of atoms at a time, but not any individual atom, which is, of course, the smallest piece of ordinary matter. However, there are ways, in effect, to see individual atoms or, at least, small groups of them. The device which accomplishes this is called an electron microscope.

On September 30, 1983, a new $8 million national center for electron microscopy was dedicated at DOE's Lawrence Berkeley Laboratory in California. The center is supported by the Department of Energy, and its dedication culminates nearly nine years of research, development, and construction. It contains the most advanced electron microscopes in the world, and has as its centerpiece a very special microscope; the only atomic resolution electron microscope in the United States. This instrument will be used by materials experts around the country from industry, university, and government laboratories to understand why materials behave as they do -- on the atomic level! It promises to show in greater detail than ever before, ways in which materials fail and, by extension, ways to design better computers, catalysts, for producing gasoline from coal, and ceramic materials for advanced, high-efficiency internal combustion engines. In addition, BIOPHYSICISTS WILL USE THE ATOMIC RESOLUTION MICROSCOPE TO STUDY THE BEHAVIOR OF PROTEINS; THE FUNDAMENTAL BUILDING BLOCKS OF LIFE. THE CENTER WILL ALSO SERVE TO TRAIN ADVANCE STUDENTS IN THE FIELD OF ELECTRON MICROSCOPY -- A FIELD WHERE BERKELEY ALREADY IS THE MAJOR NATIONAL LEADER.

WHAT IS AN ATOMIC RESOLUTION ELECTRON MICROSCOPE? HOW IS IT DIFFERENT FROM ORDINARY MICROSCOPES USING LIGHT? HOW SMALL AN OBJECT CAN IT SEE? THESE QUESTIONS RELATE TO THE SIZE OF ATOMS -- THE FUNDAMENTAL CONSTITUENTS FROM WHICH METALS, SUCH AS IRON, SEMICONDUCTORS, SUCH AS SILICON, OR PROTEINS ARE CONSTRUCTED. THE ARRANGEMENT (OR STRUCTURE) AND KINDS (OR CHEMISTRY) OF ATOMS, MAKING UP THESE MATERIALS DETERMINE THEIR PROPERTIES. FOR EXAMPLE, THE STRUCTURE AND CHEMISTRY OF ATOMS DETERMINE WHY CERTAIN MATERIALS ARE GOOD CONDUCTORS OF ELECTRICITY OR WHY THE MATERIAL SILICON IS USEFUL FOR MAKING SOLAR CELLS AND TRANSISTORS, OR WHY PROTEINS PROVIDE THE ESSENTIAL INGREDIENT TO LIFE. BECAUSE OF THIS INTERRELATION BETWEEN THE PROPERTIES OF MATERIALS AND THEIR CHEMICAL AND ATOMIC STRUCTURE, THE CAPABILITY TO SEE INDIVIDUAL ATOMS WILL ENABLE SCIENTISTS TO MORE COMPLETELY UNDERSTAND THE BEHAVIOR OF VARIOUS MATERIALS.

HOW BIG IS AN ATOM? AN ATOM IS TYPICALLY ABOUT FOUR ONE-BILLIONTHS OF AN INCH IN DIAMETER. TO GET SOME IDEA OF HOW SMALL THIS IS, THE SIZE OF AN ATOM IS TO THE SIZE OF A GOLF BALL, WHAT THE SIZE OF A GOLF BALL IS TO THE SIZE OF THE EARTH. IN ORDER TO SEE AN OBJECT, IT IS NECESSARY TO PROBE IT WITH LIGHT OR RADIATION WHOSE WAVELENGTH IS SMALLER THAN THE SIZE OF THE OBJECT. LIGHT WAVES USED FOR ILLUMINATION IN ORDINARY MICROSCOPES HAVE WAVELENGTHS ABOUT FIVE THOUSAND TIMES LARGER THAN AN ATOM. SO, ATTEMPTING TO SEE AN ATOM WITH ORDINARY LIGHT IS IMPOSSIBLE. IN ORDER TO SEE ATOMS, IT IS NECESSARY TO ILLUMINATE THEM WITH ELECTRONS ACCELERATED TO HIGH SPEED BY HIGH VOLTAGES. THESE HIGH SPEED ELECTRONS HAVE AN EQUIVALENT WAVELENGTH OF ABOUT ONE ONE-HUNDREDTH THE SIZE OF AN ATOM. THESE SMALL WAVELENGTHS ENABLE ELECTRONS TO PROBE THE ATOMS IN MATERIALS. BY MEASURING WHERE THE PROBING ELECTRONS ARE SCATTERED, IT IS POSSIBLE TO DETERMINE WHERE THE ATOMS ARE AND HOW BIG THEY ARE. THE PICTURES ARE GENERATED FROM THIS INFORMATION. THE ATOMS APPEAR AS BLACK AND WHITE DOTS ON A GRAY BACKGROUND. SINCE PROBING ELECTRONS THEMSELVES HAVE EQUIVALENT WAVELENGTHS MANY TIMES SMALLER THAN THE

DIMENSIONS OF ATOMS, IMPROVEMENTS IN THE ATOMIC RESOLUTION ELECTRON MICROSCOPE SYSTEM ITSELF MAY BRING YET UNIMAGINED FEATURES OF THE STRUCTURE OF MATERIALS INTO VIEW OF THE HUMAN EYE.

THIS CENTER IS ONE OF THE MANY FRONTIER SCIENCES FACILITIES OPERATED BY THE DEPARTMENT OF ENERGY FOR THE BENEFIT OF OUR NATION.

A JOINT GOVERNMENT AND PRIVATE INDUSTRY RESEARCH AND DEVELOPMENT EFFORT HAS PRODUCED WINNERS FOR BOTH THE NATION'S FUSION ENERGY RESEARCH PROGRAM AND THE MICROWAVE TUBE INDUSTRY. A PROGRAM MANAGED BY THE U.S. ENERGY DEPARTMENT'S OAK RIDGE NATIONAL LABORATORY WAS AIMED AT DEVELOPING A HIGH-POWER, HIGH-FREQUENCY MICROWAVE GENERATOR. AS A RESULT OF THE INDUSTRY AND NATIONAL LABORATORY INTERACTION OF THE PAST DECADE, BOTH HAVE BENEFITTED. IN THE STANDARD MICROWAVE OVEN THE MICROWAVES ARE PRODUCED BY A DEVICE CALLED A MAGNETRON. HOWEVER, FOR FUSION RESEARCH, MORE POWERFUL MICROWAVE GENERATORS ARE NEEDED. THIS NEED HAS LED TO THE DEVELOPMENT OF THE GYROTRON WHICH IS CAPABLE OF PRODUCING MUCH MORE POWERFUL MICROWAVES AT SIGNIFICANTLY HIGHER FREQUENCIES THAN FOUND IN THE HOME VERSION MICROWAVE OVEN. THIS HIGHER POWER, HIGHER FREQUENCY OUTPUT IS NEEDED TO HEAT THE PLASMA THAT IS CONTAINED IN MAGNETIC FUSION DEVICES, SUCH AS TOKAMAKS AND MIRRORS. THIS IS DONE BY HAVING THE MICROWAVES PUSH ON THE ELECTRONS IN THE PLASMA AT A FREQUENCY RELATED TO THE MAGNETIC FIELD THAT HOLDS THE PLASMA TOGETHER. THIS MAKES THE ELECTRONS OSCILLATE IN RESONANCE WITH THE MICROWAVES, MUCH LIKE PUSHING A CHILD ON A SWING. THE BIGGER THE MOTION, THE HOTTER THE PLASMA GETS. IN ORDER TO MAKE FUSION ENERGY A CANDIDATE FOR PRODUCING ELECTRICITY, A SUFFICIENTLY DENSE PLASMA OF FUSION FUEL MUST BE HEATED TO

TEMPERATURES HOTTER THAN THE SUN AND KEPT AT THOSE TEMPERATURES FOR A REASONABLE PERIOD OF TIME. MICROWAVE HEATING WITH GYROTRONS HOLDS SIGNIFICANT PROMISE IN HELPING TO ATTAIN THE REQUIRED HIGH TEMPERATURES.

MICROWAVE HEATING IN FUSION RESEARCH HAS BEEN USED SINCE THE EARLY 1970'S AND IS BEING USED INCREASINGLY.

INDUSTRIAL INVOLVEMENT BEGAN IN THE MID-1970'S, WHEN VARIAN ASSOCIATES OF PALO ALTO, CALIFORNIA, UNDERTOOK A STUDY OF THE DEVELOPMENT OF HIGH-POWER GYROTRON MICROWAVE GENERATORS FOR OAK RIDGE NATIONAL LABORATORY. FUSION ENERGY DIVISION STAFF OF THE LABORATORY REALIZED THAT THEIR PLASMA CONFINEMENT EXPERIMENT HAD FREQUENCY AND POWER REQUIREMENTS THAT EXCEEDED EXISTING TECHNOLOGY. IN 1976, VARIAN DEVELOPED A LARGE EFFICIENT GYROTRON WHILE UNDER CONTRACT TO OAK RIDGE NATIONAL LABORATORY. THREE YEARS LATER, VARIAN PRODUCED AN EVEN HIGHER POWERED DEVICE. TODAY, THEY ARE CURRENTLY INVOLVED IN CONCEPTUAL STUDIES OF STILL HIGHER-POWER, HIGHER-FREQUENCY GYROTRONS.

Hughes Aircraft Company of Torrance, California, and Raytheon Microwave Tube Division, Waltham, Massachusetts, have also been active in gyrotron studies and development.

As a result of their work for the Oak Ridge National Laboratory, both Varian and Hughes are now marketing gyrotrons. Cost of the units is between $150,000 and $300,000 each.

All of the commercial units sold to date have been for fusion experiments, although gyrotrons applications in other areas, such as isotope separation are being explored.

Gyrotrons also are being used or planned for use to heat plasmas at DOE's Princeton Plasma Physics Laboratory, at GA Technologies, San Diego, and at the Lawrence Livermore National Laboratory. U.S.-made gyrotrons are in use in fusion experiments in England, Italy, Germany, and Japan.

Future gyrotron developments will be aimed at larger fusion experiments operating at higher magnetic fields. This will require increasingly higher frequency and power. It is anticipated that Princeton's Plasma Fusion Test Reactor and other future large fusion devices will require gyrotron heating power in the tens of megawatts, with frequencies as high as 160 gigahertz.

Many of the Department of Energy's research programs have led to commercial products. This is but one example of how DOE's science programs benefit our nation.

FUSION ENERGY IS RELEASED WHEN THE NUCLEI OF THE HYDROGEN ISOTOPES, TRITIUM AND DEUTERIUM, ARE MADE TO COLLIDE WITH EACH OTHER AT A HIGH ENOUGH SPEED FOR THEM TO FUSE AND FORM HELIUM. A SIMILAR FUSION PROCESS IS WHAT POWERS OUR SUN, EXCEPT IN THE SUN, IT IS THE HYDROGEN THAT UNDERGOES A NUCLEAR FUSION REACTION. THIS SO CALLED NUCLEAR FUSION FIRE IN OUR SUN IS POSSIBLE BECAUSE THE RIGHT CONDITIONS OF EXTREMELY HIGH TEMPERATURE AND HIGH PRESSURE ARE CREATED BY THE SIZE OF THE SUN AND THE FORCE OF GRAVITY THAT HOLDS IT TOGETHER.

SINCE 1952, SCIENTISTS IN THE UNITED STATES, AND ELSEWHERE IN THE WORLD, HAVE BEEN TRYING TO DEMONSTRATE THAT CONTROLLED THERMONUCLEAR FUSION CAN TAKE PLACE IN THE LABORATORY. THEIR OBJECTIVE IS TO MAKE A PRACTICAL ENERGY SOURCE OF THE FUSION PROCESS AND USE THE RELEASED ENERGY TO GENERATE ELECTRICITY, OR SUPPLY SOME OTHER ENERGY NEED. THE PAYOFF IN THIS RESEARCH STEMS FROM THE FACT THAT THE DEUTERIUM FUEL OF A FUSION REACTOR IS EASILY OBTAINED FROM WATER AND, IN ANY PRACTICAL ENERGY RESOURCE SENSE, IS LIMITLESS. THERE ARE SOME OTHER ADVANTAGES OF FUSION THAT I WON'T GO INTO.

UNFORTUNATELY, MAKING A PRACTICAL FUSION REACTOR HAS PROVED TO BE A BIT MORE DIFFICULT THAN SCIENTISTS ORIGINALLY THOUGHT IT WAS GOING TO BE. THE PROBLEM IS THAT IT IS NECESSARY TO CREATE THE RIGHT TEMPERATURE AND PRESSURE CONDITIONS TO LIGHT THE NUCLEAR FUSION FIRE AND KEEP IT BURNING.

WITH AN ORDINARY LOG FIRE, IT IS NECESSARY TO INITIALLY HEAT THE LOGS TO A HIGH ENOUGH TEMPERATURE TO GET THEM TO IGNITE, AND THEN TO HAVE ENOUGH LOGS IN THE FIRE TO KEEP IT BURNING. IN MANY RESPECTS, IT IS THE SAME WITH FUSION, EXCEPT THAT THE TEMPERATURE HAS TO BE 100 MILLION DEGREES, AND THERE MUST BE ENOUGH FUSION FUEL HELD IN PLACE AT THIS TEMPERATURE LONG ENOUGH FOR IT TO BURN IN THE NUCLEAR SENSE. THAT IS, ENOUGH DEUTERIUM AND TRITIUM NUCLEI HAVE TO FUSE AND RELEASE MORE ENERGY THAN WAS NEEDED TO CREATE THE RIGHT CONDITIONS OF TEMPERATURE AND PRESSURE REQUIRED TO CAUSE SCIENTIFIC BREAKEVEN BY THE SCIENTISTS WORKING IN THE FIELD, AND IT IS OBVIOUSLY A NECESSARY FIRST STEP.

A COUPLE OF YEARS AGO, SCIENTISTS AT THE DEPARTMENT OF ENERGY'S PRINCETON PLASMA PHYSICS LABORATORY USED AN EXPERIMENTAL DEVICE CALLED THE PRINCETON LARGE TORURS, OR PLT, TO CONFINE AND HEAT AN IONIZED GAS, OR AS IT IS PROPERLY CALLED, A PLASMA OF DEUTERIUM NUCLEI, TO A TEMPERATURE OF ABOUT 80 MILLION DEGREES. THIS EXPERIMENT DEMONSTRATED THAT IT WAS POSSIBLE TO CREATE A PLASMA AT A HIGH ENOUGH TEMPERATURE TO LIGHT THE NUCLEAR FUSION FIRE, BUT THE PLT DEVICE COULDN'T HOLD ENOUGH FUEL LONG ENOUGH TO RESULT IN A SUSTAINED BURN.

Now, as to what's been in the news. Scientists at the Department of Energy's Fusion Studies Center at the Massachusetts Institute of Technology used another experimental device called the Alcator C to demonstrate that it is possible to hold on to, or confine, a plasma with enough fusion fuel, long enough so that a sustained burn could occur in principle, but unfortunately, their apparatus could not simultaneously produce the required high temperature. Even so, this result is an important milestone in fusion research. An essential ingredient in their success was the fuel injection apparatus they used. It makes small pellets of frozen deuterium and fries them at high speed into the plasma. This method improved plasma confinement. The Deuterium pellet injection apparatus was made at the Department of Energy's Oak Ridge National Laboratory. So now, both of the minimum conditions of temperature and confinement of a hot fusion plasma have been separately demonstrated in the laboratory. Next, it is necessary to obtain both these conditions in the same experimental apparatus. This should occur within the next two years in a device called the Tokamak Fusion Test Reactor, or TFTR for short. This TFTR, which is located at Princeton, was first operated only last Christmas Eve. So far, it has been living up

TO, OR EXCEEDING, OUR EXPECTATIONS. ALTHOUGH THERE IS MUCH TO BE DONE BEFORE FUSION MIGHT BE A PRACTICAL ENERGY SOURCE, THE RESULTS OBTAINED BY THE MASSACHUSETTS INSTITUTE OF TECHNOLOGY GROUP CLEARLY DEMONSTRATES THAT ONE OF THE IMPORTANT FUSION MILESTONES HAS BEEN PASSED.

Human cells collectively have between 30,000 and 50,000 distinct proteins. These proteins are the building blocks of life. In particular, they are precisely constructed from coded information in DNA, which contains the genetic code. That is, they are the functional machinery of cells that make up living matter. Actually, only a few percent of human proteins have been isolated and studied, and only a fraction of one percent can be measured clinically. Proteins have a wide variety of shapes and sizes. It is possible to separate these proteins one from another in a unique way using their size and shape to sort them. Without getting too technical, imagine that we could take a representative collection of human proteins from a tissue sample, and separate those that are the most spherical on the left of a sheet and those that are the most elongated on the right, and at the same time, have those that are the largest near the top of the sheet and those that are smallest near the bottom. This is actually accomplished by a process called two-dimensional gel electrophoresis, which moves each protein, depending on its size and shape, to a separate location on a sheet of specially prepared material called a gel. Present technology limits the array of separated proteins that can be identified on the gel sheet to about

100 BY 100, WHICH IS TO SAY ABOUT TEN THOUSAND SPOTS. EACH OF THESE SPOTS, WHICH ARE MADE UP OF THOUSANDS OF STAINED PROTEINS, ARE ABOUT A MILLIMETER ACROSS.

WHY IS THIS PROCESS OF BEING ABLE TO SEPARATE PROTEINS SO IMPORTANT? WELL, IT TURNS OUT THAT EACH OF US HAVE CERTAIN UNIQUE CHARACTERISTICS, SUCH AS OUR FINGERPRINTS, THAT SEPARATES US FROM EVERY OTHER HUMAN BEING. THE SAME UNIQUENESS HOLDS FOR THESE TWO-DIMENSIONAL PROTEIN MAPS. EVEN IDENTICAL TWINS WILL HAVE DIFFERENT PROTEIN MAPS. WHAT'S MORE IMPORTANT IS THAT WE CAN USE THESE PROTEIN MAPS AS RESEARCH TOOLS NOW, AND AS POSSIBLE CLINICAL TOOLS TO ROUTINELY DIAGNOSE DISEASES IN THE FUTURE. FOR INSTANCE, MOST HUMAN DISEASES, AND THE DEGENERATIVE ASPECTS OF AGING, RESULT FROM CHANGES IN THE FUNCTION, AMOUNT, OR LOCATION OF OUR PROTEINS. THESE CHANGES CAN BE DETECTED BY MEANS OF PROTEIN MAPPING. THIS LEADS TO CONSIDERATION OF THE POSSIBILITY OF OBTAINING PROTEIN MAPS FROM MANY INDIVIDUALS AND COMPARING THE MAPS TO DETERMINE IF THERE IS A CONNECTION BETWEEN THE PRESENCE OR ABSENCE OF SOME PROTEIN, OR GROUP THEREOF, AND A PARTICULAR DISEASE, OR THE SUSCEPTIBILITY TO CERTAIN DISEASES, AILMENTS, TOXIC CHEMICAL AGENTS, OR RADIATION.

Accumulating such data into a useful format is called developing a Human Protein Index. Making such an index is obviously a formidable task, and much work needs to be done before it might be practical. The reason that it is possible to consider this at all stems from several unrelated developments and advances. First, and most essential, was the development of the two-dimensional gel electrophoresis protein separation and staining methods. Second, there is the automatic scanning apparatus that can read a page of material, such as one of these gel sheets, and transfer the information into a computer memory quickly, accurately, and reproducibly. Third, there is the development of large-scale computers with large memories that can store and process these date and present the information to the scientists in a useful form. The date reduction problems are formidable, and considerable work needs to be done to extract the relevant few patterns from the millions of possibilities.

Although this project is in its early exploratory phases, good progress has been made by various groups of scientists that now use two=dimensional gel techniques. One group at DOE's Argonne National Laboratory is working to marry the scanning and computer technology to the protein maps and begin the

WORK OF DEVELOPING A HUMAN PROTEIN INDEX. OTHER DOE SCIENTISTS USE THESE PROTEIN MAPS TO DETERMINE WHAT RISKS MIGHT BE ASSOCIATED WITH THE PRODUCTION OR USE OF ENERGY , AND WHAT STEPS TO TAKE TO REDUCE THE RISK TO ACCEPTABLE LEVELS.

A SUPERCOMPUTER IS THE MOST POWERFUL COMPUTER AVAILABLE AT ANY TIME FOR DOING SCIENTIFIC CALCULATIONS. TODAY'S SUPERCOMPUTERS CAN DO MORE THAN 100 MILLION ARITHMETIC OPERATIONS PER SECOND. IT WOULD TAKE ABOUT 20 PEOPLE WORKING FULL TIME FOR A YEAR WITH HAND CALCULATORS TO DO THE SAME NUMBER OF CALCULATIONS AS A SUPERCOMPUTER DOES IN A SECOND. WHILE THIS COMPUTATIONAL POWER SEEMS ENORMOUS TODAY, IT WILL UNDOUBTEDLY BE COMMONPLACE IN TOMORROW'S "SMALL" COMPUTERS, AND THE SUPERCOMPUTER OF THE FUTURE WILL BE EVEN MORE POWERFUL.

THE MAJOR USE OF SUPERCOMPUTER IS TO SOLVE VERY LARGE SCIENTIFIC PROBLEMS IN A SHORT TIME. BY LARGE, I MEAN PROBLEMS THAT ARE MUCH TOO LARGE TO BE SOLVED ON A TYPICAL OFFICE COMPUTER, AND ARE COMPLETELY INTRACTABLE WITH PAPER AND PENCIL. THIS ENORMOUS PROBLEM SOLVING CAPABILITY ALLOWS SCIENTISTS AND ENGINEERS TO MODEL COMPLEX PROBLEMS, SUCH AS THE AIR FLOW AROUND AN AIRPLANE. IF THE MODELING CAN BE DONE WITH SUFFICIENT ACCURACY, THEN EXPENSIVE AND CONSUMING EXPERIMENTAL TESTING, SUCH AS WIND TUNNEL TESTS OF A NEW AIRPLANE DESIGN, CAN BE SIGNIFICANTLY REDUCED.

THERE ARE TWO U.S. COMPANIES THAT PRODUCE SUPERCOMPUTERS TODAY. THESE ARE CRAY RESEARCH AND CONTROL DATA CORPORATION. THESE TWO COMPANIES, WORKING WITH THE U.S. DEPARTMENT OF ENERGY, HAVE MADE THE UNITED STATES THE LEADER IN SUPERCOMPUTERS.

SUPERCOMPUTERS ARE USED FOR MAY COMPLEX SCIENTIFIC AND ENGINEERING APPLICATIONS. FOR EXAMPLE, PREDICTING WEATHER IS A COMPLEX PROBLEM FOR WHICH A NUMBER OF SUPERCOMPUTERS ARE USED TODAY, BOTH HERE IN THE U.S. AND IN EUROPE. NATIONAL AERONAUTIC AND SPACE ADMINISTRATION USES SUPERCOMPUTERS TO DESIGN AIRCRAFT AND SPACECRAFT, AND IN SOME CASES, TO SUPPLEMENT OR EVEN REPLACE WIN TUNNEL TESTING. IN THE DEPARTMENT OF ENERGY'S LABORATORIES, SUPERCOMPUTERS ARE USED FOR FUSION RESEARCH, DESIGN OF NUCLEAR WEAPONS, REACTOR SAFETY, AND FOR RESEARCH IN ENERGY SCIENCES. IN FUSION RESEARCH, COMPUTER MODELING HAS BECOME A NECESSITY. FUTURE LARGE FUSION EXPERIMENTS WILL COST HUNDREDS OF MILLIONS OF DOLLARS AND TAKE 5-7 YEARS TO BUILD. THEREFORE, IT IS NOT POSSIBLE TO BUILD VERY MANY EXPERIMENTAL DEVICES, AND COMPUTER MODELING MUST BE USED TO ENSURE THAT THE RIGHT DESIGN CHOICES ARE MADE.

INDUSTRIAL USE OF SUPERCOMPUTERS IS GROWING RAPIDLY BECAUSE THE LARGE ECONOMIC GAIN ASSOCIATED WITH APPLYING THEM TO ENGINEERING PROBLEMS. FOR EXAMPLE, ECONOMIC BENEFITS ARE BEING REALIZED BY THE PETROLEUM INDUSTRY WHERE SUPERCOMPUTERS ARE USED TO AID IN OIL EXPLORATION AND IN ELECTRONICS INDUSTRY WHERE COMPUTERS ARE USED TO DESIGN INTEGRATED CIRCUITS. IN THE

AUTOMOBILE INDUSTRY, IT HAS BEEN ESTIMATED THAT THE USE OF SUPERCOMPUTERS FOR MECHANICAL DESIGN, SIMULATED CRASH TESTING, AND SIMULATED AERODYNAMIC TESTING COULD REDUCE THE TIME REQUIRED TO DESIGN A NEW CAR BY 30%, OR ABOUT ONE YEAR.

PERHAPS ONE OF THE MORE INTERESTING USED OF SUPERCOMPUTERS IS NOT IN SCIENCE OR ENGINEERING AT ALL, BUT IN THE MAKING OF MOVIES. COMPUTER DRAWN GRAPHICS ARE NOW BEING USED TO PRODUCE SCENES FROM SCIENCE FICTION FILMS LIKE "TRON". WITH OVER 1000 HIGH QUALITY IMAGES REQUIRED FOR EACH MINUTE OF FILM, IT IS EASY TO SEE WHY A VERY POWERFUL COMPUTERS IS REQUIRED FOR THIS PURPOSE.

HISTORICALLY, SUPERCOMPUTERS HAVE ONLY BEEN USED BY SCIENTISTS IN A VERY FEW LABORATORIES. IN OTHER WORDS, THE MARKET FOR THESE MACHINES HAS BEEN SMALL. WHY THEN ARE SUCH COMPUTERS DEVELOPED? THE DEPARTMENT OF ENERGY'S LABORATORIES, PARTICULARLY THE LOS ALAMOS NATIONAL LABORATORY AND THE LAWRENCE LIVERMORE NATIONAL LABORATORY, HAVE CAUSED SEVERAL GENERATIONS OF SUPERCOMPUTERS TO BE DEVELOPED. THE PRIMARY DRIVING FORCE HAS BEEN THE NEED TO DESIGN NUCLEAR WEAPONS. THESE LABORATORIES HAVE WORKED WITH THE VENDORS TO DESIGN COMPUTERS TO TEST THEM AND TO DEVELOP THE SOFTWARE NECESSARY TO

MAKE THEM INTO USEFUL TOOLS. THEREFORE, THE DEPARTMENT HAS PLAYED A KEY ROLE IN THE DEVELOPMENT OF SUPERCOMPUTERS AND IN MAKING THE UNITED STATES THE LEADER IN THIS IMPORTANT FIELD OF TECHNOLOGY.

IT'S BEEN SAID THAT WE ARE IN THE MIDDLE OF THE COMPUTER REVOLUTION. WHILE THAT MAY APPEAR TO BE TRUE, I DON'T BELIEVE THAT THE COMPUTER REVOLUTION HAS EVEN STARTED. THIS IS TRUE FOR BOTH THE BIG SUPERCOMPUTERS AS WELL AS FOR SMALLER COMPUTERS. SUPERCOMPUTERS ARE THE BIGGEST AND FASTEST COMPUTERS AVAILABLE. THEY ARE CAPABLE OF DOING OVER 100 MILLION ARITHMETIC OPERATIONS PER SECOND. THIS SEEMS LIKE AN ENORMOUS COMPUTING CAPABILITY, HOWEVER, BY THE END OF THE DECADE, WE ARE GOING TO NEED COMPUTERS THAT ARE AT LEAST 100 TIMES FASTER THAN THOSE CURRENTLY AVAILABLE.

HOW WILL THE DEVELOPMENT OF THESE MORE ADVANCED COMPUTERS PROCEED, AND HOW WILL SCIENTISTS AND ENGINEERS USE THEM? TO SOME EXTENT, THE DEVELOPMENT WILL BE DRIVEN BY OUR NEED TO SOLVE PROGRESSIVELY MORE COMPLEX SCIENTIFIC AND TECHNICAL PROBLEMS. THEIR UTILIZATION WILL BE DETERMINED BY HOW READILY ACCESSIBLE THESE NEW SUPERCOMPUTERS ARE AND HOW MUCH THEY WILL COST TO OPERATE.

FROM THE EARLIEST DAYS OF COMPUTING UP TO THE PRESENT, MOST COMPUTERS HAVE SOLVED PROBLEMS BY DOING THE REQUIRED CALCULATIONS ONE AFTER ANOTHER. TO DO PROBLEMS FASTER, IT IS NECESSARY TO DO THE INDIVIDUAL CALCULATIONS FASTER. THUS, THE GREAT INCREASES IN COMPUTER PERFORMANCE IN THE LAST 30 YEARS HAVE

PRIMARILY BEEN ACHIEVED BY IMPROVEMENTS IN THE ELECTRONIC COMPONENTS USED TO BUILD COMPUTERS. YESTERDAY'S VACUUM TUBES WERE SLOW. TODAY'S MODERN INTEGRATED CIRCUITS ARE MUCH FASTER. COMPUTING SPEED INCREASES OF OVER 1000 TIMES HAVE BEEN OBTAINED BY THE USE OF BETTER COMPONENTS, BUT IT DOES NOT APPEAR THAT ANOTHER FACTOR OF 1000 CAN BE OBTAINED THIS WAY. THERE IS ANOTHER LIMITATION ON HOW FAST COMPUTERS CAN BE MADE TO OPERATE. IT HAS TO DO WITH THE FACT THAT IT TAKES TIME FOR AN ELECTRONIC SIGNAL TO GET FROM POINT A TO POINT B IN A COMPUTER. THE LENGTH OF TIME IS DETERMINED BY THE SPEED THAT A SIGNAL MOVES ALONG THE LENGTH OF WIRE BETWEEN THESE POINTS. THAT SPEED IS THE SPEED OF LIGHT WHICH IS A FIXED CONSTANT OF NATURE AND CANNOT BE INCREASED. SINCE THERE IS A LIMIT TO HOW SHORT CONNECTING WIRES CAN BE MADE, THERE IS A LIMIT ON HOW FAST ELECTRONIC SYSTEMS CAN BE MADE TO OPERATE. THIS MEANS THAT THERE MUST BE A NEW APPROACH TO COMPUTER DESIGN IF THEY ARE TO BE MADE TO OPERATE AT HIGHER COMPUTING SPEEDS. UNE NEW APPROACH IS TO HAVE THE COMPUTER WORK ON MORE THAN ONE PART OF A PROBLEM AT THE SAME TIME. THIS IS EQUIVALENT TO HAVING SEVERAL COMPUTERS WORK IN CONCERT ON THE SAME CALCULATION. YOU MIGHT THINK THAT ARBITRARY INCREASES IN COMPUTER PERFORMANCE MIGHT BE ACHIEVED BY SIMPLY EXTENDING THIS IDEA TO EQUIVALENTLY

PUT MORE AND MORE COMPUTERS TO WORK ON THE SAME CALCULATION. NOT THAT EASY. IN PRACTICE, IT'S QUITE DIFFICULT TO HAVE MANY COMPUTERS WORK IN PARALLEL ON THE SAME PROBLEM. THIS IS REALLY A FUNDAMENTALLY NEW WAY TO BUILD COMPUTERS. MUCH RESEARCH AND DEVELOPMENT WILL BE REQUIRED TO MAKE IT SUCCESSFUL.

SINCE THE SUPERCOMPUTER IS SUCH AN IMPORTANT SCIENTIFIC TOOL, IT IS ESSENTIAL THAT THE UNITED STATES NOT LOSE ITS LEADERSHIP IN THIS FIELD. COMPUTERS PLAY VITAL ROLES IN OUR NATIONAL SECURITY EFFORTS, AS WELL AS BEING IMPORTANT FOR SCIENTIFIC RESEARCH, AND THE DEVELOPMENT OF NEW PRODUCTS, SUCH AS AUTOMOBILES, AIRPLANES, ELECTRONICS, AND EVEN MOVIES.

FOR SUPERCOMPUTERS TO BE USED TO HELP ADVANCE OUR KNOWLEDGE IN THESE VARIOUS FIELDS OF SCIENCE AND TECHNOLOGY, THEY HAVE TO BE MADE MORE AVAILABLE TO MANY RESEARCHERS IN UNIVERSITIES, LABORATORIES, AND INDUSTRY. UP UNTIL NOW, SUPERCOMPUTERS HAVE BEEN AVAILABLE TO ONLY A RELATIVELY FEW SCIENTISTS AND ENGINEERS. ONE OF THE REASONS IS THEIR COST. THEY RUN ABOUT TEN MILLION DOLLARS EACH, AND IT COSTS QUITE A BIT TO KEEP THEM OPERATING. FOR THIS REASON, IT IS NOT PRACTICAL FOR EACH UNIVERSITY OR LABORATORY TO HAVE THEIR OWN SUPERCOMPUTER. FORTUNATELY, WITH MODERN COMMUNICATIONS, A COMPUTER USER

DOES NOT NEED TO BE LOCATED NEAR THE COMPUTER. INSTEAD, THE USER COMMUNICATES WITH THE COMPUTER THROUGH TELEPHONE LINES OR SATELLITE LINKS USING A TERMINAL THAT IS MUCH LIKE A HOME COMPUTER.

TEN YEARS AGO, THE DEPARTMENT OF ENERGY ESTABLISHED A COMPUTER CENTER AND COMMUNICATIONS NETWORK TO SERVE ITS MAGNETIC FUSION ENERGY PROGRAM. TODAY, THIS NETWORK HAS TWO SUPERCOMPUTERS LOCATED AT DOE'S LAWRENCE LIVERMORE NATIONAL LABORATORY. THESE SUPERCOMPUTERS ARE ACCESSED BY OVER 2000 FUSION SCIENTISTS AND ENGINEERS WHO ARE GEOGRAPHICALLY DISPERSED ALL OVER THE COUNTRY. BOTH SATELLITE AND TELEPHONE COMMUNICATIONS ARE USED TO CONNECT THEM TO THE LIVERMORE COMPUTERS. THE NETWORK BEING USED BY THE FUSION PROGRAM HAS SHOWN THAT LARGE SCALE SCIENTIFIC COMPUTING CAN BE DONE IN AN EFFICIENT AND COST EFFECTIVE MANNER. I EXPECT THAT SUCH REMOTE USE OF SUPERCOMPUTERS WILL BE THE PATTERN OF THE FUTURE.

THROUGHOUT THE CENTURIES, HUMANS HAVE ASKED, "WHERE IS MY MIND?", "HOW DOES MY MIND WORK?", AND "WHAT CAUSES MY MIND TO WORK POORLY OR BECOME DISEASED?" AS SCIENCE PROGRESSED, THE FOCUS OF THESE QUESTIONS BECAME THE HUMAN BRAIN IN BOTH ITS NORMAL AND ITS DISEASED CONDITION. EVEN TODAY, WE ARE STILL LOOKING FOR A GREATER UNDERSTANDING OF THESE QUESTIONS. MANY OF THE KEYS TO UNLOCK THESE SECRETS, ESPECIALLY THOSE OF THE THOUSANDS OF COMPLEX CHEMICAL PROCESSES, FUNCTIONS, AND MALFUNCTIONS GOING ON IN THE BRAIN, ARE BEING PROVIDED BY RESEARCH SPONSORED BY THE DEPARTMENT OF ENERGY.

BASIC RESEARCH, WHICH OFTEN HAS NO INITIALLY RECOGNIZED, PRACTICAL APPLICATION, CAN PRODUCE KNOWLEDGE AND TURN IT INTO TOOLS OF GREAT POWER THAT CAN BRING ABOUT PROGRESS IN INDUSTRY, IN MEDICINE, AND IN OTHER FIELDS, FOR THE BENEFIT OF ALL.

TWO SUCH TOOLS HAVING GREAT IMPORTANCE TO THE STUDY OF THE BRAIN ARE CHEMICAL COMPOUNDS LABELED WITH POSITRON EMITTING ATOMS AND THE POSITRON EMISSION TOMOGRAPH, OR PET SCANNER. WITH THESE TOOLS, SCIENTISTS AND PHYSICIANS CAN ACCURATELY TRACK THE DISTRIBUTION AND CONSUMPTION OF BIOCHEMICALS IN THE HUMAN BODY BY SIMPLE ADMINISTRATION OF THE RADIOACTIVELY

LABELED TRACER MOLECULES, THROUGH EITHER INHALATION OR INJECTION. THESE RADIOACTIVELY LABELED FORMS OF NATURAL SUBSTANCES ACTUALLY PARTICIPATE IN THE BRAIN'S CHEMICAL PROCESSES. TOMOGRAPHY INVOLVES THE USE OF A COMPUTER MEMORY THAT STORES INFORMATION PROVIDED BY AN ARRAY OF DETECTORS THAT DETERMINE THE NUMBER OF POSITRON EMITTING ATOMS AT EACH LOCATION IN THE BRAIN. THIS COMPUTER THEN PROCESSES THE INFORMATION AND GIVES THE PHYSICIAN OR RESEARCHER A COLOR TELEVISION PICTURE THAT SHOWS WHICH PARTS OF THE BRAIN ARE ACTIVE.

THE PET SCANNER STORY BEGAN THREE DECADES AGO WHEN THE FOUNDATIONS FOR THE METHODS WERE BEING LAID BY THE STUDY OF THE CHEMISTRY OF SHORT-LIVED ATOMS WHICH DECAY BY EMITTING POSITRONS. MUCH OF THIS EARLY WORK OCCURRED AT DOE'S BROOKHAVEN NATIONAL LABORATORY. IT MADE POSSIBLE THE PREPARATION OF MANY OF TODAY'S RADIOACTIVELY LABELED COMPOUNDS.

POSITRON EMISSION IS A TYPE OF RADIOACTIVE DECAY THAT ALLOWS DETERMINATION OF THE QUANTITY AND LOCATION OF THE TAGGED COMPOUNDS. THESE COMPOUNDS ARE PRODUCED BY BOMBARDING CERTAIN GASES AND LIQUIDS WITH ELEMENTARY PARTICLES, SUCH AS PROTONS OR NEUTRONS COMING FROM AN ACCELERATOR. THE COMPOUNDS HAVE SHORT LIFETIMES; A FEW MINUTES TO A FEW MONTHS. THEY CANNOT BE STORED, AND MUST BE PRODUCED AT OR NEAR THE SITE WHERE THEY ARE TO BE USED.

In 1976, chemists at Brookhaven National Laboratory worked with a team at the University of Pennsylvania Medical School and the National Institutes of Health to develop a method that uses a labeled glucose tracer and positron emission tomography, to measure the level of metabolic activity of glucose in the brain. Glucose and Oxygen combine to provide the brain's major source of energy. The PET brain scans show where, and how rapidly, Glucose is being utilized. Physicians are already using PET scans to measure the brain's metabolic activity in stroke victims, epilepsy, and other serious disorders of the brain. Still, perhaps among the most exciting ventures on the horizon for positron emission tomography is the study of mental illnesses, such as schizophrenia, depression, and senile dementia--diseases that afflict a significant proportion of our society. Distinctive patterns of biochemical activity have begun to emerge, holding promise for more accurate diagnosis and treatment of some of society's most puzzling and debilitating ailments.

Today's research efforts are proceeding well beyond the measurement of Glucose metabolic activity. Chemists are preparing substances that can probe the brain's ability to transmit information, its reaction to and use

OF OPIATES AND ITS ABILITY TO SYNTHESIZE PROTEINS. THE GROWTH RATE OF TUMORS OF THE BRAIN CAN ALSO BE MEASURED. BASIC TO ALL OF THESE IS HOW THE BRAIN'S CHEMISTRY CONTROLS LEARNING, BEHAVIOR, AND MENTAL CONDITION. IN 1976, THERE WERE ONLY THREE PET CENTERS, ALL OF THEM IN THE UNITED STATES. TODAY, THERE ARE SEVERAL DOZEN AROUND THE WORLD.

RESEARCH EFFORTS ARE DIRECTED NOT ONLY TOWARDS INCREASED USE IN BIOLOGICAL AND MEDICAL RESEARCH, BUT TO AUTOMATING AND SIMPLIFYING THE TECHNOLOGY SO THAT ITS BENEFITS CAN BECOME EVEN MORE WIDESPREAD. THE DEPARTMENT OF ENERGY CONTINUES TO SUPPORT AND ENCOURAGE THE UNDERLYING CHEMICAL AND BIOLOGICAL BASIC RESEARCH AND HIGH TECHNOLOGY, WHICH IS NECESSARY FOR SUCCESS IN THIS EMERGING FIELD.

THE DEPARTMENT OF ENERGY SUPPORTS A VARIETY OF PROJECTS IN SEVERAL AREAS OF BASIC RESEARCH. SOME OF THESE HAVE LED TO IMPORTANT APPLICATIONS AND COMMERCIAL PROJECTS. ONE INTERESTING EXAMPLE INVOLVES THE SO-CALLED AMORPHOUS SOLIDS. GLASS IS AN AMORPHOUS SOLID. THAT IS, WHEN A PIECE OF GLASS IS BROKEN, THERE IS NO OBVIOUS STRUCTURE. HOWEVER, WHEN A PIECE OF METAL, SUCH AS IRON IS BROKEN, THERE IS AN OBVIOUS CRYSTALLINE STRUCTURE THAT APPEARS AT THE BREAK. THIS STRUCTURE IS FORMED AS THE IRON COOLS FROM A MOLTEN STATE TO A SOLID STATE. IT HAS A DOMINATE EFFECT ON THE STRENGTH OF THE IRON AND ON OTHER PROPERTIES, SUCH AS ELECTRICAL CONDUCTIVITY AND MAGNETISM.

THE REASON THAT METALS HAVE THIS CRYSTALLINE OR GRAIN STRUCTURE HAS TO DO WITH THE WAY THE METAL ATOMS ARRANGE THEMSELVES IN PERIODIC ARRAYS IN SOLIDS. ABOUT 25 YEARS AGO, PROFESSOR POL DUWEZ AT CAL TECH WAS STUDYING THE PROPERTIES OF METALS FOR DOE'S PREDECESSOR AGENCY, THE ATOMIC ENERGY COMMISSION. HE WISHED TO REDUCE THE SIZE OF THE GRAINS THAT FORMED IN METALS. TO DO THIS, HE TRIED COOLING MOLTEN METAL SO FAST THAT GRAIN GROWTH WOULD BE INHIBITED. WHAT HE DID WAS TO SQUIRT A SMALL STREAM OF MOLTEN METAL ON TO A RAPIDLY SPINNING COLD METAL WHEEL. THIS PROCESS PRODUCED A

THIN METAL STRIP THAT WAS A METAL, BUT DIDN'T HAVE CRYSTALLINE STRUCTURE. THAT IS, IT WAS AMORPHOUS-LIKE GLASS. HENCE, THE POPULAR TERM FOR SUCH MATERIALS; NAMELY, GLASSY METALS.

THIS WAS THE BEGINNING OF A FIELD OF RESEARCH THAT HAS IMPORTANT APPLICATIONS. I WILL OUTLINE ONE OF THESE APPLICATIONS AND ITS IMPORTANCE TO ENERGY SAVINGS.

IT TURNS OUT THAT THE ABSENCE OF GRAIN STRUCTURE IS IMPORTANT IN TERMS OF THE MAGNETIC PROPERTIES OF METALS.

IF A PIECE OF IRON IS SUBJECTED TO A MAGNETIC FIELD THAT IS CHANGING ITS DIRECTION RAPIDLY, THE IRON IS HEATED, ESSENTIALLY BECAUSE THE GRAINS RUB AGAINST EACH OTHER AS THEY CHANGE DIRECTION WITH THE MAGNETIC FIELD. THIS IS ONE OF THE CAUSES OF ENERGY LOSS THAT OCCURS IN THE MILLIONS OF POWER TRANSFORMERS THAT ARE USED BY COMPANIES TO BRING ELECTRICITY INTO OUR HOMES AND FACTORIES. AN AMORPHOUS SOLID OR GLASSY METAL DOESN'T HAVE THIS PROBLEM BECAUSE THERE ARE NO GRAINS. SINCE ABOUT ONE-FOURTH OF THE ENERGY CONSUMED ANNUALLY IN THE UNITED STATES IS ASSOCIATED WITH ELECTRICAL GENERATION, ANY SAVINGS OF LOSSES IS OBVIOUSLY IMPORTANT. FOR EXAMPLE, IF THE 20 MILLION

DISTRIBUTION TRANSFORMERS IN THE UNITED STATES WERE REPLACED WITH ONES THAT HAD AN AMORPHOUS SOLID CORE, ABOUT 12 BILLION KILOWATT-HOURS OF ENERGY WOULD BE SAVED EACH YEAR. THIS IS ABOUT THE ENERGY USED BY A CITY OF 4 MILLION PEOPLE. OBVIOUSLY, WE CAN'T GO AROUND AND REPLACE ALL THE EXISTING TRANSFORMERS, BUT WE COULD BEGIN TO USE THEM FOR SOME OF THE ONE MILLION NEW DISTRIBUTION TRANSFORMERS INSTALLED EACH YEAR.

THE GENERAL ELECTRIC COMPANY WILL BUILD ABOUT 1000 OF THESE TRANSFORMERS. THE ELECTRIC POWER RESEARCH INSTITUTE, WHO IS CO-SPONSORING THIS PROGRAM, WILL IN TURN DISTRIBUTE THEM TO UTILITIES AS PART OF A FIELD TESTING PROGRAM.

ALTHOUGH MUCH WORK NEEDS TO BE DONE TO IMPROVE PRODUCTION TECHNIQUES BEFORE THESE TRANSFORMERS WITH GLASSY METAL CORES CAN BE USED EXTENSIVELY, IT IT CLEARLY A GOOD BEGINNING.

AS WITH ANY NEW TECHNOLOGY, VARIOUS APPLICATIONS ARE BEING EXPLORED. TAPE RECORDER PLAYBACK HEADS AND STARTING CIRCUITS FOR FLOURESCENT LIGHTS ARE AMONG THEM.

AMORPHOUS METALS ARE CERTAINLY GOING TO FIND THEIR WAY INTO MANY IMPORTANT APPLICATIONS. THEY ARE A GOOD EXAMPLE OF HOW THE DEPARTMENT OF ENERGY'S BASIC RESEARCH PROGRAMS LEAD TO APPLICATIONS OF IMPORTANCE TO OUR NATION.

WHAT IS A QUARK?

WHAT IS A LEPTON?

MORE PEOPLE ARE LEARNING TO USE THESE WORDS ALL THE TIME. SOME OF THEM ARE HIGH SCHOOL STUDENTS FROM THE CHICAGO AREA. SCIENCE ORIENTED JUNIORS AND SENIORS SPENT ABOUT 3 TEN-WEEK SESSIONS STUDYING AND UNDERSTANDING PHYSICS. THEY ARE LEARNING ABOUT QUARKS AND LEPTONS FROM SOME OF THE WORLD'S LEADING SCIENTISTS AT DOE'S FERMILAB. THIS LAB, WHICH IS LOCATED ABOUT 30 MILES WEST OF CHICAGO, IS NAMED IN HONOR OF ENRICO FERMI, THE NOBEL LAUREATE, WHO BUILT THE FIRST ATOMIC REACTOR AT THE UNIVERSITY OF CHICAGO IN 1942. THESE FERMILAB SCIENTISTS VOLUNTEER THEIR TIME TO TEACH PROMISING HIGH SCHOOL STUDENTS SOME OF THE FUNDAMENTALS OF HIGH ENERGY PHYSICS. THE PROGRAM, WHICH WAS FOUNDED 4 YEARS AGO, HAS GRADUATED MORE THAN 900 STUDENTS, MANY OF WHOM HAVE GONE ON TO SEEK HIGHER EDUCATION IN MATH AND PHYSICS. THE INCREASING POPULARITY HAS MADE IT DIFFICULT TO ACCOMMODATE ALL THE INTERESTED AND QUALIFIED STUDENTS. TO MAKE INFORMATION PRESENTED AT THESE SATURDAY LECTURES MORE AVAILABLE TO THE INTERESTED STUDENTS AND THE GENERAL PUBLIC, THE AURORA FOUNDATION IN ILLINOIS HAS MADE A GRANT OF $12,800 TO THE FRIENDS OF FERMILAB ASSOCIATION TO PRODUCE AND DISTRIBUTE VIDEO TAPES OF THE FERMILAB SATURDAY MORNING PHYSICS LECTURES.

WHY IS THIS IMPORTANT? IT TURNS OUT THAT ONE OF THE GREATEST CHALLENGES OF ANY RESEARCH ORGANIZATION IS TO DISSEMINATE THE KNOWLEDGE GAINED THROUGH THEIR RESEARCH. TRADITIONALLY, KNOWLEDGE IS EXCHANGED BY RESEARCHERS AND OTHER INTERESTED INDIVIDUALS AT PROFESSIONAL MEETINGS AND THROUGH JOURNAL ARTICLES AND INFORMAL COLLEAGUE COLLABORATION NETWORKS. OUR RESEARCHERS ARE ACTIVELY ENGAGED IN THESE ACTIVITIES. THESE METHODS, HOWEVER, ARE PRIMARILY AIMED AT THE RESEARCHERS THEMSELVES. THE TIME REQUIRED FOR THE INFORMATION TO TRICKLE DOWN TO EDUCATORS WITH A TRUE UNDERSTANDING OF THE KNOWLEDGE IS UNACCEPTABLE IN AN AGE OF EVER-INCREASING TECHNOLOGY KNOWLEDGE AND INCREASING PUBLIC SENSITIVITY TO THE IMPACT OF TECHNOLOGY ON SOCIETY. DOE'S LABORATORIES, INCLUDING FERMILAB, ARE NOW LOOKING TO BYPASS THIS TRICKLE DOWN PROCESS AND GO DIRECTLY TO HIGH SCHOOL FACULTY AND STUDENTS. SOME OF THESE OTHER DOE LABORATORY ACTIVITIES CONSIST OF ACTUAL PARTICIPATION IN ONGOING RESEARCH BY FACULTY AND STUDENTS, LECTURES AND SEMINARS, AND MOTIVATIONAL ACTIVITIES TO ENCOURAGE STUDENTS TO CONSIDER A CAREER IN SCIENCE OR ENGINEERING. THIS LARGELY VOLUNTEER EFFORT BY DOE SCIENTISTS IS VERY SUCCESSFUL.

IN THE BEGINNING, I STARTED WITH THE QUESTION - WHAT ARE QUARKS AND LEPTONS?. THE SIMPLE ANSWERS IS THAT THEY ARE SOME OF THE BUILDING BLOCKS OF ATOMS THAT SCIENTISTS ARE STILL LEARNING ABOUT. ATOMS, IN TURN, ARE THE BUILDING BLOCKS OF ORDINARY MATTER THAT SURROUND US. LEPTON IS THE WORD THAT SCIENTISTS USE TO DESCRIBE A CLASS OF SUBATOMIC PARTICLES OF WHICH AN ELECTRON IS THE MOST FAMILIAR. THE OTHER PARTS OF AN ATOM ARE THE PROTON AND NEUTRON WHICH MAKE UP ITS NUCLEUS. IN THE LAST FEW YEARS, IT HAS BEEN SHOWN THAT THE PROTON AND NEUTRON HAVE QUARKS AS THEIR BUILDING BLOCKS. THIS ISN'T THE END OF THE STORY FROM A SCIENTIFIC POINT OF VIEW. PHYSICISTS AT FERMILAB AND OTHER LABORATORIES CONTINUE TO WORK ON AN UNDERSTANDING OF HOW THE LESS FAMILIAR SUBATOMIC PARTICLES ARE BUILD OF QUARKS. THESE SATURDAY LECTURES MAKE IT POSSIBLE FOR THESE SCIENTISTS TO SHARE THEIR SENSE OF EXCITEMENT IN THE CHALLENGE OF UNDERSTANDING THESE MOST FUNDAMENTAL PARTS OF MATTER.

IF YOU CONNECT A PIECE OF WIRE BETWEEN THE TERMINALS OF A BATTERY, THE WIRE BEGINS TO WARM UP. THE REASON THAT THE WIRE GETS HOT IS THAT THE CURRENT OF ELECTRONS FLOWING IN IT EXPERIENCE A FORM OF ELECTRICAL FRICTION, WHICH IS CALLED RESISTANCE. BY CONTROLLING THE RESISTANCE OF THE WIRES, WE CAN MAKE ELECTRICAL SPACE HEATERS, ELECTRIC LIGHT BULBS, TOASTERS, AND SO ON. IN THESE CASES, ELECTRICAL RESISTANCE IS A USEFUL PROPERTY THAT WE PUT TO PRACTICAL USE. HOWEVER, IN MANY CASES, THIS SAME RESISTANCE RESULTS IN AN UNDESIRABLE LOSS OF ELECTRIC POWER. FOR INSTANCE, IT DOES NO GOOD TO HEAT THE AIR ALONG THE THOUSANDS OF MILES OF WIRES THAT BRING ELECTRIC POWER INTO OUR HOMES AND FACTORIES. ONE AREA WHERE THIS LOSS OF ELECTRIC POWER IS PARTICULARLY SERIOUS IS IN THE OPERATION OF ELECTROMAGNETS. THE STRENGTH OF THE FIELD PRODUCED BY AN ELECTROMAGNET IS DETERMINED BY ITS CURRENT. UNFORTUNATELY, HEATING OF THE ELECTROMAGNET, DUE TO ITS ELECTRICAL RESISTANCE, WOULD CAUSE IT TO BURN OUT, IF THE CURRENT WERE INCREASED TO THE LEVELS NEEDED TO PRODUCE THE STRONG MAGNETIC FIELDS REQUIRED FOR CERTAIN RESEARCH AND INDUSTRIAL APPLICATIONS.

THERE IS A SOLUTION TO THE PROBLEM. IT TURNS OUT THAT WHEN WE COOL A SUBSTANCE, ITS ELECTRICAL RESISTANCE BECOMES SMALLER. HOWEVER, FOR MOST MATERIALS THERE IS A TEMPERATURE BELOW WHICH ELECTRICAL RESISTANCE CEASES TO REDUCE. FORTUNATELY, THERE ARE SOME SUBSTANCES THAT HAVE A UNIQUE PROPERTY CALLED SUPERCONDUCTIVITY, WHICH OCCURS WHEN THEY ARE COOLED TO A FEW DEGREES ABOVE ABSOLUTE ZERO, WHICH IS 273 DEGREES CELSIUS BELOW ZERO.

THIS PHENOMENON WAS DISCOVERED IN 1911 BY A DUTCH SCIENTISTS NAMED KAMERLINGH ONNES. HE FOUND THAT THE ELEMENT MERCURY LOSES ALL TRACES OF ELECTRICAL RESISTANCE WHEN COOLED TO NEAR ABSOLUTE ZERO. THAT IS, IT BECOMES A SUPERCONDUCTOR, A TERM HE COINED.

FOR MANY YEARS THE PHENOMENON OF SUPERCONDUCTIVITY REMAINED A LABORATORY CURIOSITY. DURING THIS PERIOD, IT WAS FOUND THAT MANY OTHER METALS AND ALLOYS, AS WELL AS CERTAIN POLYMERS, BECOME SUPERCONDUCTING AT TEMPERATURE BELOW 25 DEGREES ABOVE ABSOLUTE ZERO. NOW, THERE HAVE EMERGED SOME IMPORTANT APPLICATIONS OF SUPERCONDUCTIVITY, AND OTHERS WILL BE COMING ALONG IN THE FUTURE.

THE DEPARTMENT OF ENERGY HAS PIONEERED IN THE DEVELOPMENT OF NEW AND IMPROVED SUPERCONDUCTING MATERIALS AND THEIR APPLICATIONS. ONE APPLICATION THAT IS PARTICULARLY NOTEWORTHY IS THE SO CALLED ENERGY SAVER PROGRAM AT DOE'S FERMILAB. IN ORDER TO MAKE A MODERN HIGH ENERGY PHYSICS PARTICLE ACCELERATOR, STRONG MAGNETIC FIELDS ARE REQUIRED TO STEER THE BEAM OF PARTICLES IN A CIRCULAR PATH WHILE THEY ARE BEING ACCELERATED. LATE LAST YEAR, FERMILAB STARTED OPERATION OF THE WORLD'S FIRST ACCELERATOR USING SUPERCONDUCTING MAGNETS. THE AVAILABILITY AND PRICE OF ELECTRICAL POWER, AND THE TECHNOLOGY OF CONVENTIONAL WATER COOLED COPPER MAGNETS MAKES IT IMPRACTICAL TO USE FERMILAB'S EXISTING 4 MILE CIRCUMFERENCE TUNNEL TO ACCELERATE PARTICLES TO MORE THAN ONE HALF TERAELECTRON VOLT, OR TEV AS IT IS USUALLY REFERRED TO. ONE TEV IS ONE MILLION MILLION ELECTRON VOLTS. THE NEW SUPERCONDUCTING MAGNETS USE ONLY A FRACTION OF THE ELECTRICAL POWER OF CONVENTIONAL MAGNETS. THE STRONGER FIELD OF THE SUPERCONDUCTING MAGNETS PERMITS ACCELERATION OF PARTICLES TO MORE THAN ONE TEV WHICH WILL NEARLY DOUBLE THE ACCELERATORS PEAK ENERGY TO A NEW WORLDS RECORD. SCIENTISTS AT THE DOE'S LAWRENCE LIVERMORE NATIONAL LABORATORY HAVE BUILT AND OPERATED THE WORLD'S LARGEST SUPERCONDUCTING MAGNET FOR USE IN FUSION RESEARCH. THIS

MAGNET WEIGHS MORE THAN 750,000 POUNDS AND STANDS MORE THAN 14 FEET HIGH.

AT THE OAK RIDGE NATIONAL LABORATORY, THE LARGE COIL TEST FACILITY WAS BUILT TO TEST SIX LARGE SUPERCONDUCTING COILS ARRANGED TO MAKE A TOROIDAL FIELD FOR FUSION RESEARCH. THREE OF THESE SIX COILS ARE SUPPLIED AS PART OF AN INTERNATIONAL COOPERATION INVOLVING JAPAN, GERMANY, AND SWITZERLAND.

A PHENOMENON KNOWN AS NUCLEAR MAGNETIC RESONANCE, OR NMR, IS NOW BEING USED TO MAKE NON-INVASIVE MEASUREMENTS OF PARTS OF THE HUMAN BODY. THIS TECHNIQUE REQUIRES STRONG MAGNETIC FIELDS OVER VOLUMES THE SIZE OF HUMANS. SUPERCONDUCTING MAGNETS ARE THE ANSWER NOT ONLY FOR COST BUT ALSO FOR THE FACT THAT THE MAGNETIC FIELD CAN BE MADE TO HAVE THE REQUIRED UNIFORMITY AND STEADINESS.

IN THE FUTURE, ELECTRICAL GENERATORS, ELECTRIC STORAGE SYSTEMS, TRANSFORMERS, AND POWER TRANSMISSION SYSTEMS WILL LIKELY USE SUPERCONDUCTING TECHNOLOGY. SOME HAVE ALREADY BEEN BUILT AND TESTED. DOE'S SUPPORTED RESEARCH IN FUSION, HIGH ENERGY PHYSICS, AND MATERIALS PROPERTIES HAS BEEN A KEY FACTOR IN BRINGING THIS IMPORTANT TECHNOLOGY INTO PRACTICAL APPLICATION.

AS WE GROW OLDER, OUR JOINTS BEGIN TO DETERIORATE. FOR THE MOST PART, THIS IS JUST A NUISANCE THAT SLOWS SOME OF US UP A LITTLE OR RESTRICTS OUR ACTIVITIES IN SOME MINOR WAYS. HOWEVER, IN SOME CASES, THE DETERIORATION IS MORE SERIOUS AND IS ACCOMPANIED BY GREAT PAIN AND LOSS OF IMPORTANT MOBILITY. WHETHER IT IS FROM INJURY, AGING, OR SOME CONDITION LIKE ARTHRITIS DOESN'T MATTER TO THE VICTIM. WHAT DOES MATTER IS OBTAINING RELIEF. EACH YEAR MORE THAN 75,000 AMERICANS ARE FITTED WITH SURGICALLY IMPLANTED ARTIFICIAL HIP JOINTS. THIS RESTORES THEIR MOBILITY AND PROVIDES RELIEF FROM THE PAIN OF WORN OR DISEASED JOINTS. UNFORTUNATELY, EVEN THESE ARTIFICIAL HIP JOINTS WEAR OUT, AND SOME HAVE TO BE REPLACED. THE NATURAL MOTION OF WALKING BEGINS TO REMOVE SOME OF THE PROTECTIVE OXIDES OF THE METAL ALLOY "BALL" AS IT MOVES IN THE POLYETHYLENE HIP "SOCKET". THIS PERMITS THE CORROSIVE BODY FLUIDS TO ATTACK THE EXPOSED METAL. THIS, IN TURN, INTRODUCES UNDESIRABLE METALLIC IONS IN THE BODY. THE REMOVED OXIDE PARTICLES BECOME IMBEDDED IN THE POLYETHYLENE AND CONTINUE TO SCRATCH THE BALL, THUS PRODUCING MORE METALLIC DEBRIS, WHICH SHORTENS THE USEFUL LIFE OF THE "JOINT".

SCIENTISTS AT THE DEPARTMENT OF ENERGY'S OAK RIDGE NATIONAL LABORATORY AND THE UNIVERSITY OF ALABAMA AT BIRMINGHAM RECENTLY REPORTED A MATERIALS ADVANCE THAT PROMISES TO INCREASE THE USEFUL LIFE OF THESE ARTIFICIAL

HIP JOINTS BY MORE THAN 400 TIMES. THIS WOULD MAKE THEM GOOD FOR THE LIFETIME OF THE RECIPIENT, THUS ELIMINATING THE NEED FOR A SECOND REPLACEMENT. THE MATERIALS ADVANCE INVOLVES MODIFYING THE WORKING SURFACE OF THE ARTIFICIAL JOINT'S LIGHT WEIGHT TITANIUM ALLOY BALL. THE TECHNIQUE, KNOWN AS "ION IMPLANTATION", PLACES A THIN LAYER OF NITROGEN ATOMS IN THE OUTER SURFACE OF THE BALL. THIS SMALL QUANTITY OF NITROGEN HAS A MAJOR EFFECT ON THE SURFACE. IT MAKES IT EXTREMELY RESISTANT TO MECHANICAL WEAR AND BODY FLUID CORROSION. THIS MINIMIZES THE RELEASE OF METALLIC PARTICLES THAT MAY CONTRIBUTE TO THE PAINFUL TISSUE INFLAMATION THAT IS SOMETIMES ASSOCIATED WITH ARTIFICIAL HIP JOINTS.

ION IMPLANTATION IS JUST ONE OF SEVERAL SURFACE MODIFICATION TECHNIQUES NOW BEING USED IN MATERIALS SCIENCE RESEARCH. SURFACE MODIFICATION TECHNIQUES ARE IMPORTANT BECAUSE FEW ALLOYS HAVE BOTH THE DESIRED BULK PROPERTIES AND SURFACE CHARACTERISTICS NEEDED FOR A PARTICULAR APPLICATION. THIS IS THE CASE WITH THE ARTIFICIAL HIP JOINTS WHERE THE ALLOY MUST BE CAREFULLY SELECTED FOR ITS BULK AND FATIGUE STRENGTH, AS WELL AS WEIGHT, TO TAKE THE IMPACT STRESS CAUSED BY WALKING. WITH SURFACE MODIFICATION TECHNIQUES, ENGINEERS CAN CHOOSE THE ALLOY FOR ITS BULK PROPERTIES AND THEN MODIFY THE SURFACE TO GIVE IT THE PROPER CORROSION OR WEAR CHARACTERISTICS FOR A PARTICULAR APPLICATION.

LIKE MANY MODERN TECHNOLOGY APPLICATIONS, ION IMPLANTATION OWES ITS EXISTENCE TO MANY PREVIOUS, APPARENTLY UNRELATED DEVELOPMENTS AND DISCOVERIES. KEY AMONG THEM IN THIS CASE IS THE EARLY WORK IN NUCLEAR PHYSICS. IN ORDER TO STUDY THE NUCLEUS OF THE ATOM, SCIENTISTS NEEDED ACCELERATORS THAT COULD BRING ATOMS TO HIGH SPEEDS AND FIRE THEM INTO TARGETS WHERE SOME OF THE ATOMS WOULD BE SPLIT. THESE SAME ACCELERATORS ARE NOW BEING USED TO FIRE CERTAIN ATOMS, SUCH AS NITROGEN IN THE CASE OF HIP JOINTS, INTO TARGETS WHERE THEY PENETRATE A FEW ATOMIC DIAMETERS AND MODIFY THE SURFACE STRUCTURE OF THE TARGET.

THE HIP JOINT ION IMPLANTATION WAS DONE AT THE COLLABORATIVE RESEARCH CENTER FOR SURFACE MODIFICATION AT OAK RIDGE NATIONAL LABORATORY. THE INVESTIGATION OF THE CORROSION AND WEAR RESISTANCE WAS DONE AT THE UNIVERSITY OF ALABAMA, BIRMINGHAM. THIS COLLABORATION IS ANOTHER EXAMPLE OF HOW DOE'S LABORATORIES WORK WITH UNIVERSITY SCIENTISTS TO TRANSFER THE BENEFITS OF BASIC AND APPLIED RESEARCH FROM THE LABORATORY TO THE PUBLIC.

YOU HAVE NO DOUBT HEARD OF THE EXPRESSION "A MIND IS A TERRIBLE THING TO WASTE." OUR NATION CAN'T AFFORD TO WASTE ANY OF ITS TALENT. THIS MEANS THAT WE MUST DO WHAT WE CAN TO ENSURE THAT ALL OF OUR PEOPLE RECEIVE GOOD TRAINING AND EDUCATION. THE DEPARTMENT OF ENERGY PLAYS AN IMPORTANT ROLE IN THE TRAINING OF SCIENTISTS AND ENGINEERS THROUGH ITS RESEARCH AND DEVELOPMENT CONTRACTS IN AREAS OF SCIENCE AND TECHNOLOGY RELATED TO ITS MISSION. THIS USUALLY INVOLVES ADVANCED TRAINING OR GRADUATE STUDIES ASSOCIATED WITH RESEARCH IN THE PHYSICAL SCIENCES, CHEMISTRY, LIFE SCIENCES, AND NUCLEAR MEDICINE APPLICATIONS. IN A MUCH SMALLER WAY, THE DEPARTMENT IS ALSO INVOLVED IN PROGRAMS THAT SEEK TO ENCOURAGE YOUNGER STUDENTS TO PURSUE CAREERS IN THESE AREAS BY HAVING THEM PARTICIPATE IN SATURDAY SEMINARS AT SOME OF OUR NATIONAL LABORATORIES AND BY WORKING ON SUMMER PROJECTS AT SOME OF THESE SAME LABORATORIES.

ONE OF THESE PROGRAMS, CALLED PREP, FOR PREFRESHMEN ENGINEERING PROGRAM, INVOLVES 20 UNIVERSITY-BASED PROJECTS THAT SEEK OUT MINORITY AND WOMEN STUDENTS WHO ARE INTERESTED IN, BUT NOT COMMITTED TO, SCIENTIFIC OR TECHNICAL CAREERS. OF THE 1500 STUDENTS THAT PARTICIPATE IN THIS PROGRAM EACH YEAR, MORE THAN 75% GO ON TO COLLEGE. ALSO, OVER 90% OF THE 300 MINORITY HIGH SCHOOL STUDENTS THAT WORK IN RESEARCH APPRENTICESHIP PROGRAMS AT FIVE OF OUR NATIONAL LABORATORIES GO ON TO COLLEGE EACH YEAR.

ANOTHER AREA WHERE THE DEPARTMENT IS INVOLVED IN IS WITH THE HISTORICALLY BLACK COLLEGES. THIS IS INPART A RESULT OF THE EXECUTIVE ORDER BY PRESIDENT REAGAN DIRECTING FEDERAL AGENCIES TO SIGNIFICANTLY INCREASE SUPPORT FOR THESE HISTORICALLY BLACK COLLEGES. HOWEVER, EVEN BEFORE THIS ORDER, THE DEPARTMENT WAS INVOLVED IN SOME RESEARCH PROGRAMS AT SOME OF THESE INSTITUTES. JUST RECENTLY, I ATTENDED A CEREMONY DEDICATING A LABORATORY FOR LASER CHEMISTRY RESEARCH AT HOWARD UNIVERSITY IN THE DISTRICT OF COLUMBIA. THIS IS AN EXCELLENT PROGRAM SUPPORTED BY GRANTS FROM SEVERAL AGENCIES. THE DOE WORK INVOLVES THE USE OF LASERS TO STUDY THE CHEMICAL BONDING OF CARBON AND NITROGEN, WHICH IS IMPORTANT IN THE UNDERSTANDING OF ENERGY CONVERSION PROCESSES.

THE POSSIBILITY OF USING LASER CHEMISTRY TO EXTRACT TRACE QUANTITIES IN THE FEW PARTS PER BILLION RANGE OF HIGHLY TOXIC SUBSTANCES FROM WATER IS ALSO BEING EXPLORED AT HARVARD. THIS INVOLVES TONING THE LASER COLOR TO A FREQUENCY ABSORBED BY THE TOXIC SUBSTANCE. THIS IN TURN CHANGES ITS CHEMICAL NATURE IN SUCH A WAY THAT IT CAN BE EASILY FILTERED OUT.

IN A COMPLETELY DIFFERENT FIELD OF ENERGY RESEARCH, SCIENTISTS AT TUSKEGEE INSTITUTE IN ALABAMA, ARE LOOKING AT THE PHYSIOLOGICAL AND BIOCHEMICAL

EFFECTS OF ATMOSPHERIC CARBON DIOXIDE TO HELP US MODEL THE POTENTIAL EFFECTS OF ITS INCREASE ON OUR FOOD CROPS. IN ANOTHER PROJECT, SUPPORTED BY OUR FUSION ENERGY PROGRAM, SCIENTISTS AT ATLANTA UNIVERSITY ARE INVOLVED IN COOPERATIVE FUSION ENGINEERING RESEARCH WITH SCIENTISTS AT THE DEPARTMENT OF ENERGY'S OAK RIDGE NATIONAL LABORATORY. THE DEPARTMENT OF ENERGY'S LAWRENCE BERKELEY LABORATORY HAS ESTABLISHED A COOPERATIVE RESEARCH AND EDUCATION PROGRAM WITH JACKSON STATE UNIVERSITY IN MISSISSIPPI. THIS PROGRAM INVOLVES STUDENT AND FACULTY INTERNSHIPS AT BERKELEY AS WELL AS ASSISTANCE IN THE DEVELOPMENT OF NEW COURSES AND RESEARCH PROGRAMS AT THE JACKSON STATE CAMPUS. A SIMILAR COOPERATIVE PROGRAM HAS BEEN INITIATED BETWEEN ATLANTA UNIVERSITY AND THE DEPARTMENT OF ENERGY'S ARGONNE. BOTH THESE PROGRAMS EMPHASIZE "ONE ON ONE" RELATIONSHIPS BETWEEN SCIENTISTS AT THE LABS AND FACULTY AND STUDENTS AT THE PARTICIPATING UNIVERSITIES--THE BEST WAY, WE FEEL, TO HELP STRENGTHEN THE CAPABILITIES OF BOTH FACULTY AND STUDENTS TO CONTRIBUTE IN ADVANCED ENERGY RESEARCH.

THESE ARE BUT A FEW OF THE DEPARTMENT'S PROGRAMS THAT SEEK TO EXPAND THE POOL OF TRAINED SCIENTISTS AND ENGINEERS TO INCLUDE ALL SEGMENTS OF OUR SOCIETY.

EB: Dr. Trivelpiece, I understand that the Department has just selected five scientists to receive some special awards. Could you explain what this is all about?

AT: Secretary of Energy, Don Hodel, recently presented five awards to recognize outstanding achievement in the field of atomic energy. These awards were established in 1959 to honor the memory of Nobel Laureate Dr. Ernest Orlando Lawrence. Dr. Lawrence invented the cyclotron. This invention led to the huge accelerators that are used by today's high energy physicists. These devices are not only the largest, but they are also the most sophisticated research tools of modern science. Cyclotrons are also used today to treat patients in hospitals, and to make radioisotopes for patient treatment and diagnosis.

It was to recognize the great importance of Dr. Lawrence's contributions, that President Eisenhower approved the establishment of these awards in 1958. The awards recognize the achievements of scientists, who are early in their careers, and who have already demonstrated outstanding scientific and technical accomplishments in fields related to atomic energy. The awardees must also show exceptional promise of future achievement.

THE FIRST OF THE FIVE AWARDEES IS DR. JAMES JACKSON. HE IS A NUCLEAR ENGINEER AT DOE'S LOS ALAMOS NATIONAL LABORATORY IN NEW MEXICO. HE WAS SELECTED FOR HIS RESEARCH ON THE SAFETY OF NUCLEAR REACTORS. DR. JACKSON DEVELOPED WAYS TO USE COMPUTERS TO ANALYZE POSSIBLE ACCIDENTS IN THE TYPES OF REACTORS WE HAVE TODAY. HE THEN EXTENDED THESE METHODS TO APPLY THEM TO FAST BREEDER REACTORS, SHOWING THAT THEY WILL BE SAFER THAN HAD BEEN PREVIOUSLY ASSUMED.

ANOTHER AWARDEE, DR. MICHAEL PHELPS IS A NUCLEAR CHEMIST IN THE SCHOOL OF MEDICINE AT UCLA IN CALIFORNIA. HE WAS A MAJOR PARTICIPANT IN DEVELOPING POSITRON EMISSION TOMOGRAPHY, USUALLY CALLED PET. PET SCANNERS ALLOW RESEARCHERS TO OBSERVE HOW BLOOD FLOWS IN THE BRAIN, HOW THE BRAIN USES ENERGY, AND HOW THESE THINGS CHANGE AS A RESULT OF BRAIN-RELATED DISEASE. THE PET SCANNER DEPENDS ON THE USE OF SPECIALLY PREPARED CHEMICAL COMPOUNDS, INCLUDING RADIOACTIVE ATOMS, WHICH ARE MADE WITH THE AID OF A CYCLOTRON. DR. PHELPS DEVELOPED MANY OF THE PET SCANNER TECHNIQUES THAT ARE USED IN HOSPITALS.

DR. PAUL RUTHERFORD IS A PLASMA PHYSICIST AT DOE'S PRINCETON PLASMA PHYSICS LABORATORY IN NEW JERSEY. HE HAS MADE MAJOR CONTRIBUTIONS TO OUR PROGRESS OF UNDERSTANDING HOW TO OBTAIN ENERGY FROM CONTROLLED FUSION. FUSION ENERGY CAN BE RELEASED WHEN A PLASMA OF LIGHT NUCLEI, SUCH AS DEUTERIUM, IS HEATED TO TEMPERATURES HOTTER THAN THE INTERIOR OF THE SUN. THE ONLY WAY TO CONFINE SUCH A PLASMA IS WITH INTENSE MAGNETIC FIELDS. DR. RUTHERFORD DEVELOPED INGENIOUS COMPUTER MODELS TO DESCRIBE HOW HOT PLASMA BEHAVES AND INTERACTS WITH SUCH MAGNETIC FIELDS. HE THEN USED THESE MODELS TO HELP DESIGN A SUCCESSION OF MAJOR EXPERIMENTAL DEVICES THAT HAVE BEEN USED TO STUDY FUSION PLASMAS.

DR. MARK WRIGHTON IS A CHEMIST AT THE MASSACHUSETTS INSTITUTE OF TECHNOLOGY. ALTHOUGH HE IS ONLY 34 YEARS OLD, HE HAS ALREADY PUBLISHED OVER 50 SCIENTIFIC PAPERS, MAKING MAJOR CONTRIBUTIONS TO THE FIELD OF PHOTOCHEMISTRY. HIS RESEARCH EXPLORES HOW LIGHT CAN CHANGE THE PROPERTIES OF COMPLICATED MOLECULES. THIS FUNDAMENTAL RESEARCH HAS A HOST OF POTENTIAL PRACTICAL APPLICATIONS. THESE INCLUDE: BATTERIES, FUEL CELLS, AND POSSIBLY A WHOLE NEW CLASS OF SOLAR CELLS TO MAKE ELECTRICITY FROM SUNLIGHT.

Mr. George Zimmerman is a physicist at DOE's Lawrence Livermore National Laboratory in California. He has made important strides in computational physics. His special achievement has been to describe and dissect the many effects that take place when a tiny pellet of nuclear fusion fuel is suddenly bombarded with beams of laser light or particles. This process has the potential of leading to a miniature nuclear explosion. This might make it possible to study nuclear weapons phenonomen without using underground nuclear explosions. It may also someday lead to a practical new source of energy. Mr. Zimmerman's calculations are the heart of this work.

In a ceremony at DOE Headquarters in Washington, Secretary Hodel presented these Lawrence Award winners a citation, a gold medal, and a check for $5,000. I am sure that Dr. Lawrence would be proud of the accomplishments of these awardees, who are helping to create the new scientific knowledge that will shape our future.

THE AMAZING NEUTRON (PART 1)

A LITTLE OVER 50 YEARS AGO A BRITISH SCIENTIST NAMED CHADWICK MADE A REMARKABLE DISCOVERY. HE FOUND THAT IN ADDITION TO ELECTRONS AND PROTONS, ATOMS CONTAINED A THIRD KIND OF PARTICLE CALLED A NEUTRON. THE NEUTRON IS ELECTRICALLY NEUTRAL. IT IS MADE UP OF AN ELECTRON AND A PROTON, TO WHICH IT DECAYS IN ABOUT 15 MINUTES WHEN IT IS FREE AND OUTSIDE THE NUCLEUS OF AN ATOM. COMBINATIONS OF NEUTRONS AND PROTONS MAKE UP THE CORE OR NUCLEUS OF ATOMS OF MATTER. FOR INSTANCE, HYDROGEN HAS ONE PROTON IN ITS NUCLEUS, WHILE HELIUM HAS 2 PROTONS AND 2 NEUTRONS.

WE ARE ALL FAMILIAR WITH HOW X-RAY'S PENETRATE MATTER AND CAN BE USED TO TAKE PICTURES OF THE INSIDE OF OUR BODY. IN A SENSE, X-RAY'S SEE THE ELECTRONS OF THE ATOMS THAT MAKE UP MATERIAL OBJECTS. IT TURNS OUT THAT A BEAM OF NEUTRONS CAN BE USED TO OBTAIN A PICTURE OF THE INTERIOR OF OBJECTS. THE DIFFERENCE IS THAT THE NEUTRON TENDS TO SEE PROTONS RATHER THAN ELECTRONS. THIS, COMBINED WITH THE FACT THAT THE ELECTRICALLY NEUTRAL NEUTRON EASILY PENETRATES MATTER, MAKES IT A POWERFUL TOOL FOR SCIENTISTS TO USE IN STUDYING THE PROPERTIES OF MATTER.

It permits scientists to probe, without harming the sample, the nature of the binding forces within interesting and important materials. These observations help us to understand, for example, why diamond is so hard and nearly indestructible, while other elements, such as copper, are softer and can easily be deformed into many varied useful shapes.

Even though neutrons only live for 15 minutes, this is a sufficiently long time to perform interesting experiments. A few of the very heavy elements, such as uranium, have an overabundance of neutrons in the nucleus and they can be unleashed by the fission process, whereby a neutron splits the atom, creating even more neutrons. This is the principle of the DOE research reactors at DOE 's Oak Ridge and Brookhaven National Labs, which produce some of the most intense neutron beams in the world. Neutrons can also be produced by particle bombardment of suitable targets in accelerators. This is being done at the DOE labs at Livermore, Argonne, Los Alamos, and Oak Ridge. The unwanted neutrons are absorbed by heavy shielding and the useful neutrons are extracted through tubes in the shielding for experimental purposes.

THE FIELD OF MEDICINE HAS BENEFITTED ENORMOUSLY FROM THE UNIQUE PROPERTIES OF THE NEUTRON. BECAUSE THE NEUTRON CAN PENETRATE THE NUCLEUS OF MANY ELEMENTS, IT CAN CAUSE A TRANSMUTATION OF THE NUCLEUS INTO A NEW SPECIES. THAT IS, IT ALLOWS US TO MAKE SPECIAL ATOMS. SOME ARE RADIOACTIVE AND CAN BE USED FOR DIAGNOSIS AND TREATMENT OF DISEASES. FOR EXAMPLE, IN DIAGNOSIS THE MOVEMENT OF RADIOISOTOPES THROUGH COMPLEX CHEMICAL AND BIOLOGICAL REACTIONS CAN BE FOLLOWED. AS A RESULT, VARIOUS TYPES OF TUMORS HAVE BEEN DETECTED IN THE BRAIN AND OTHER PARTS OF THE BODY WITH THE ASSISTANCE OF SOPHISTICATED MEDICAL INSTRUMENTATION. A WHOLE NEW INDUSTRY HAS BEEN CREATED FROM THESE FUNDAMENTAL DISCOVERIES APPLIED TO SPECIAL PROBLEMS. THERE ARE SIMILAR APPLICATIONS TO OTHER TECHNOLOGIES. DOE IS THE PRINCIPAL PRODUCER OF THESE RADIO AND STABLE ISOTOPES FOR USE IN MEDICINE AND SCIENCE.

ALTHOUGH THE NEUTRON HAS NO ELECTRICAL CHARGE, IT DOES HAVE A SMALL MAGNETIC MOMENT WHICH MAKES IT BEHAVE LIKE A TINY MAGNET. THIS PROPERTY IS VERY IMPORTANT AND PROVIDES A MOST UNIQUE PROBE OF MAGNETIC MATERIALS. DOE IS THE PRINCIPAL PROVIDER OF THESE POWERFUL NEUTRON SOURCE WHICH ARE USED AS RESEARCH TOOLS MADE AVAILABLE TO THE SCIENTIFIC COMMUNITY FOR A VARIETY OF EXPERIMENTS.

The neutron was discovered in 1932 by a British Physicist named Chadwick. Since that time, countless applications of neutrons have been developed. The first major application was the wartime development of nuclear weapons. The element uranium has a natural isotope, designated Uranium 235. This isotope has the property that a neutron can cause it to fission, release energy, and generate two or three free neutrons in the process. If enough Uranium 235 is packed to a high density, these free neutrons cause a chain reaction with consequent rapid release of energy, which is what gives rise to the destructive power of nuclear weapons. If the Uranium 235 is diluted in the right way, this chain reaction can be controlled. This means that the release of energy can be slowed down and be made to generate heat to produce steam to make electricity. This is what occurs in a nuclear reactor. More than 12% of the electricity in the United States is now supplied in this way by more than 80 operating nuclear reactors. But not all reactors are used

TO MAKE ELECTRICITY. SOME ARE DESIGNED TO PERMIT ACCESS TO A BEAM OF NEUTRONS OR CREATE AN ENVIRONMENT WITHIN THE REACTOR WHERE MATERIALS CAN BE SUBJECTED TO HIGH DOSES OF NEUTRONS. SINCE NEUTRONS HAVE NO ELECTRICAL CHARGE, THEY READILY PASS THROUGH MATERIALS. HOWEVER, IN SO DOING, SOME NEUTRONS COLLIDE WITH THE NUCLEI OF THE ATOMS IN THE SAMPLE BEING BOMBARDED.

SOMETIMES THE NEUTRON JUST SCATTERS OR BOUNCES OFF THE NUCLEUS AND GOES OFF IN SOME NEW DIRECTION. BY MEASURING THIS CHANGE OF DIRECTION, SCIENTISTS CAN LEARN ABOUT THE INTERIOR OF SOME MATERIALS. THIS PROCESS IS CALLED NEUTRON DIFFRACTION ANALYSIS. ONE OF THE RESEARCH FACILITIES WHERE THIS KIND OF WORK IS DONE IS AT THE HIGH FLUX ISOTOPE REACTOR, LOCATED AT DOE'S OAK RIDGE NATIONAL LABORATORY. A BEAM OF NEUTRONS IS EXTRACTED FROM THIS REACTOR TO DO NEUTRON DIFFRACTION MEASUREMENTS TO STUDY THE STRUCTURE OF MATERIALS. FOR EXAMPLE, THE STRENGTH OF VARIOUS STEELS, ALLOYS, AND CERAMICS ARE GREATLY INFLUENCED BY THEIR MICROSTRUCTURE. THIS MICROSTRUCTURE CAN BE INVESTIGATED WITH THE AID OF NEUTRON DIFFRACTION ANALYSIS TO ESTABLISH THE UNDERSTANDING NEEDED TO MAKE STRONGER OR TOUGHER MATERIALS.

SOME OF THE NEW ATOMIC SPECIES RESULTING FROM NEUTRON BOMBARDMENT ARE RADIOACTIVE. THEY HAVE A UNIQUE RADIATION SIGNATURE THAT CAN BE USED TO DETERMINE THEIR PRESENCE AND IDENTIFY THEM.

THIS PROPERTY HAS EVEN BEEN USED TO VERIFY THE AUTHENTICITY OF PRICELESS PAINTINGS. BY THIS NEUTRON ACTIVATION ANALYSIS, AND AUTORADIOGRAPHY, PAINTINGS BENEATH PAINTINGS, OR FORGERIES, CAN BE REVEALED.

THE NEUTRON TRANSMUTATION OF SILICON TO PHOSPHORUS IS USED EXTENSIVELY BY INDUSTRY FOR MAKING CERTAIN TYPES OF SEMICONDUCTORS FOR ELECTRONIC CIRCUITS. INGOTS OF SILICON CRYSTALS ARE IRRADIATED IN REGIONS OF HIGH NEUTRON FLUX IN THE INTERIOR OF NUCLEAR REACTORS. SOME OF THE SILICON ATOMS CAPTURE NEUTRONS AND THEN EMIT ELECTRONS AND BECOME PHOSPHORUS ATOMS. IT WOULD BE DIFFICULT, IF NOT IMPOSSIBLE, TO PREPARE THIS TYPE OF MATERIAL TO PRECISE SPECIFICATIONS IN ANY OTHER WAY, ECONOMICALLY.

NEUTRONS ARE NOW BEING USED AS WELL AS X-RAYS TO TAKE STUDY OF THE STRUCTURE OF MATERIALS. THE PENETRATING POWER OF THE NEUTRON ALLOWS SCIENTISTS TO "SEE" LIGHT ORGANIC MATERIALS INSIDE METAL CONTAINERS. FOR EXAMPLE, IT'S POSSIBLE TO OBSERVE THE DEGRADATION OF BATTERIES INSIDE A PACEMAKER, OR THE EFFECTS OF LUBRICANTS IN PREVENTING WEAR.

A FUNDAMENTAL UNDERSTANDING OF THE ELECTRONIC STRUCTURE OF MANY HIGH TECH MATERIALS, SUCH AS SUPERCONDUCTORS, HAS BEEN GREATLY ADVANCED BY OBSERVING HOW NEUTRONS SCATTER WHEN THEY RECOIL FROM COLLISIONS WITH THE NUCLEI OF ATOMS WHICH MAKE UP THESE MATERIALS. THIS BASIC KNOWLEDGE IS ALLOWING NEW MATERIALS TO BE DESIGNED AND EXISTING MATERIALS IMPROVED.

THESE ARE JUST A FEW EXAMPLES OF HOW THE NEUTRON CAN BE USED TO ADVANCE OUR TECHNOLOGY. IT WILL CONTINUE TO DO SO IN THE FUTURE. MANY OF THESE APPLICATIONS HAVE THEIR ORIGIN IN STUDIES DONE AT DOE'S NEUTRON RESEARCH FACILITIES.

Dr. TRIVELPIECE. The other thing I wanted to touch on, before coming to the BES program, involves what is called the multiprogram general purpose facilities, the MGPF program. Over the years, the laboratories have been allowed to deteriorate slightly, and that deterioration is the result of a natural kind of conflict of interest which a manager at a laboratory has to face as well as managers that work in the headquarters program. That is, in periods of budget stringencies, do you fix the roads, or do you let people go? I am afraid that in the past, the practice has been probably more than has been appropriate to let the roads go and other things like them.

DOE this year and last year has tried to put together a program in which the facilities at the laboratories pay special attention to, and we are asking for $39 million for the MGPF program this year. That will do things like fix the water chillers at Brookhaven and fix the electrical system at Oak Ridge National Laboratory, and redo the medical facility which is at Livermore which is sadly deteriorated. We are trying to be responsible and see to it that the facilities that have been brought into existence at taxpayers' expense are maintained in an adequate and proper manner.

In that regard, there is another category of funding which relates to this, which is called a GPP and GPE. That is general plant projects and general purpose equipment. Last year, the recently established Laboratory Management Council, which the Department now uses as a board of directors to look over the broad issues that relate to national laboratories, gave special attention to GPP and GPE. In fact, I have tried to increase it across the board in areas where it is important. This does not show up as a single line item in the budget, but I call your attention to it here on the grounds that we are paying special attention to that as an activity. You may notice in the budget, there is a $7 million item which is the

GPP, GPE request for Argonne National Laboratory. That was assigned to Energy Research as a landlord responsibility from the nuclear program. It is a new item in the budget, which has not been in there before.

In the remaining time in these opening remarks, I am supposed to summarize the BES program. Of course, that is some $419 million and 1,400 projects. It is not entirely clear how to do that in a few minutes, but I wanted to at least touch on a few items here.

Last year, when I appeared before you, I pointed out that the Energy Research Advisory Board had at our request undertaken a review of the national laboratories. They have made some recommendations that we should look at the laboratories as institutions and try to redirect them into newer productive activities and try to integrate them better as a partnership with the universities and with industry.

Of course, we try to do that with some initiatives which we brought forward. We are a little bit astonished at the response that occurred as a result of that, and in fact personally, I was a little bit disappointed at what I feel is a rather parochial interest on the part of some of the scientists in the United States who take a negative view of this thing.

I would like to remind everyone that in effect DOE is a mission-oriented agency, and we are not strictly like the National Science Foundation, in which there is a response to scientists wishing the facilities. We have our own internal needs, and in some cases this year with regard to things like the advanced light source, I do not think proper attention was given to some of the weapons programs' needs. I would like to have included for the record, to be submitted later, a letter from Mr. Ebert to me concerning the synchotron light sources needs of the weapons program, which is part of the mission-oriented activities that the Department is engaged in.

[The material referred to follows:]

Lawrence Livermore National Laboratory

January 3, 1984

Hon. Alvin Trivelpiece
Director of Energy Research, ER-1
U.S. Department of Energy
Washington, D.C. 20585

Dear Dr. Trivelpiece,

Enclosed for your information is a letter to Mike Knotek that expresses our dissatisfaction with the interim report from his committee. If I can provide any additional information or assistance, please let me know.

Sincerely,

Paul J. Ebert

Lawrence Livermore National Laboratory

January 3, 1984

Dr. Michael L. Knotek
Sandia National Laboratories
P. O. Box 5800
Albuquerque, NM 87185

Dear Mike,

I recently received a copy of your and Peter Eisenberger's letter to Alvin Trivelpiece, Director of Energy Research. You shouldn't be surprised to find that I strongly object to the statement of priorities and can hardly understand how the committee's recommendations could have been unanimous.

I believe that members of the committee should reconsider Walter Trela's presentation, which projected very rapid growth in the DOE Weapons Laboratories' synchrotron radiation (SR) requirements. Trela also pointed out that our SR requirements mapped almost ideally into the ALS photon spectrum and that new classes of experiments in atomic and plasma physics could only be accomplished with a source that is at least as bright as ALS. Such experiments will be essential to many ongoing programs, particularly here at LLNL, but also at LANL and Sandia.

I hope that the committee's final report will reflect our requirements as well as requirements other than in the materials science area.

Sincerely,

Paul J. Ebert

cc: P. Eisenberger
R. Kropschot
A. Trivelpiece

Dr. **Trivelpiece**. We were partially successful, even so, and I think the Nation is better off as a result. There was a package of things that were part of that initiative, and they included some upgrades to the National Synchotron Light Source, and that is proceeding, and the Stanford Synchotron Research Laboratory and those are proceeding, and some of the things that were part of the package of activities that were proposed for Berkeley are continuing: the Surface Sciences Catalysis Laboratory and the Advanced Materials Laboratory. One is not part of the appropriation we are discussing here today but was carried along as a result of this initiative, and that is the High Temperature Materials Laboratory that has been initiated at the Oak Ridge National Laboratory.

I would like to spend just a few minutes now pointing out a couple of the accomplishments. Unfortunately, all of us have the habit of growing older, and as we do, certain infirmities of age begin to appear. These include arthritis and degenerative diseases of the joints and so on. In some cases they are kind of a nuisance. In other cases, they become a downright serious problem. The problem has to do with the implantation of hip joints, and there are about 75,000 Americans a year who get a new hip joint that is an artificial one.

These things have a habit of eroding and corroding as a result of body fluids that attack the surface of the titanium that fits in the polyethylene socket. Through a cooperative research effort between the University of Alabama and the Oak Ridge National Laboratory, some of the implantation of nitrogen ions into the surface of the titanium ball has resulted in a hip joint that has a lifetime that is 400 times the lifetime of those who have been previously available. That I think is a remarkable achievement and illustrates the kind of cooperative activities that take place in some cases between our laboratories and universities.

Previously I have mentioned at hearings in this committee the materials called nickel aluminide, which was a material that does not use critical materials and yet has the property that its strength increases as a function of temperature. This was developed through the Oak Ridge National Laboratory. The reason I mention it here is, although we talked about it earlier, it was the recipient of an IR-100 award. That is a rather important award for activities to receive in the United States, in terms of their benefit to the Nation.

I would point out that the basic energy sciences program is the recipient of nine of the IR-100 awards this last year for activities that are supported directly through the program.

Another activity that occurred this year, I was going to call attention to is the dedication of the atomic resolution microscope at Berkeley, as part of the National Microscope Center. It is the first device in the United States that is actually capable of taking materials and resolving the structure of them down to the atomic level. That is a facility that will be used by industry and by the national laboratories and by universities. It is an important attribute, and it was dedicated last September 30.

I have testified before you on supercomputers, and as you are aware we have an initiative in supercomputers this year. We did propose to manage this as a separate activity, reporting to me through Dr. Jim Decker as a separate office within the Office of Energy Research. OMB did not quite see the management issue my way, and that is why the budget for that activity is carried in the basic energy sciences program. We will still manage it through Dr. Decker, but the budget is carried here. It does not reflect any diminution of our interest and desire to try to assist the Nation in its need for supercomputers, both with respect to access at universities as we have talked about on many occasions, but also the need to try to improve the acceleration of the development of the next generation of supercomputers.

At the outset of the hearing here, you mentioned the fact that the increase in the BES budget is $85 million from last year. The temptation would be to say that is not a real increase. Of course it is a real increase, but I at least wanted to go through what the elements of that are to put them into context.

This program manages many national facilities. These national facilities, some of them are new and they have just recently come into operation. In order to operate these facilities properly, just as we discussed with the high energy physics accelerators, it is important that they be utilized at a level that is consistent with their investment. Of the $85 million, $20 million is devoted to that activity.

Something like $10 million is just the ordinary cost of living. Approximately $25 million is the continuation of construction for activities that have already been authorized, $13 million is for the supercomputer initiative, and I have already mentioned $7 million, which is the GPP, GPE funds for the Argonne National Laboratory. Finally, there are some activities which have come to us as a result of some transfers. One is the heavy ion fusion program, and the other is a nuclear data program, which was originally supported through the nuclear program in the Department.

This kind of nuclear data program we have acquired the responsibility for, and I am pleased to do so because I think it is very important. As a Nation, we do not do as good a job as we should at providing dollar data and documented data in a number of areas. The critical evaluative data that are available to engineers and scientists for use in the design of powerplants is very important. Small differences in relatively subtle things like cross-sections of interaction in nuclear data can amount to matters of percents in the efficiency of operation of powerplants. That is a tremendous saving in the resources our Nation has, as well as a reduction in cost. So I think this kind of data effort is very important, and we are pleased to take it on, but it is something which has been added to our program.

Mr. Chairman, that completes the introductory remarks that I planned to make, and I would be happy to answer any questions now.

[The prepared statement of Dr. Trivelpiece follows:]

Statement of Alvin W. Trivelpiece

Director of Energy Research

Department of Energy

Mr. Chairman and Members of the Subcommittee:

I am pleased to be here today to discuss the FY 1985 budget request for the Energy Research (ER) programs under the Supporting Research and Technical Analysis budget activity within the Energy Supply R&D appropriation. These programs include: Basic Energy Sciences, Energy Research Analyses, University Research Support, University Research Instrumentation, Multiprogram General Purpose Facilities, Advisory and Oversight Program Direction and Policy and Management. These programs are listed in Table 1, which shows the total ER budget request for FY 1985. This budget request reflects the goals and strategies set out in the Fourth National Energy Policy Plan (NEPP-IV), published in October 1983. As stated in NEPP-IV, the goal of our national energy policy is to foster an adequate supply of energy at reasonable costs. The strategies for achieving this goal are: (1) to minimize Federal control and involvement in energy markets while maintaining public health and safety and environmental quality, and (2) to promote a balanced and mixed energy resource system. NEPP-IV also stresses the need to continue to advance the frontiers of our scientific and technical knowledge and provide fundamental building blocks for technological innovation.

Over the years the United States has developed a tradition of leadership in science and technology which has made us a model for developing nations throughout the world. All of our national goals -- better health and quality of life for all our people, vigorous economic growth, energy self-sufficiency, national security, space exploration, etc. -- involve technological advances that depend on basic research. The principal product of this research is knowledge, the foundation from which new ideas and concepts emerge and on which important decisions can be made.

Table 1
Office of Energy Research
Summary by Program
($ in millions)
Budget Authority

	FY 1984 Estimate	FY 1985 Request
eneral Science & Research[a]		
High Energy Physics	$480.0	$561.0
Nuclear Physics	159.0	183.6
General Science Program Direction	2.2	2.2
Subtotal	641.2	746.8
Energy Supply - R&D		
Basic Energy Sciences	$337.3	$419.5
Magnetic Fusion Energy[a]	470.8	483.1
Biological & Environmental Research[a]	183.9	189.1
Energy Research Analyses	2.9	3.0
University Research Support	5.5	9.2
University Research Instrumentation	4.0	6.0
Multiprogram General Purpose Facilities	42.1	39.0
Advisory & Oversight Program Direction	3.4	2.9
Policy and Management	1.3	0.5
Subtotal	$1,051.2	$1,152.3
Total ER	$1,692.4	$1,899.1[b]

a/ These programs are the subjects of separate hearings.

b/ These estimates reflect $15.6 million for savings resulting from FY 1985 management initiatives.

Basic research is a high-risk activity requiring long-term commitments and large sums of money with no promise of obvious success or early returns on investments. Consequently, the private sector has little incentive to support it.

The goal of the Basic Energy Sciences (BES) program is the production of scientific and engineering knowledge for use by the Government and the private sector in developing new concepts, materials and processes for use in energy exploration, production, and conversion. The knowledge that results from BES-sponsored research, thus, becomes a vital part of the body of information on which developments in the applied energy technologies rest. Basic Energy Sciences' research in the physical, biological and mathematical sciences is carried out largely by scientists at universities and national laboratories. An important benefit that results from supporting research at universities is the technology transfer that occurs when graduate students carry their knowledge of cutting edge research to their new employment environment after completion of their studies. In addition to universities and laboratories, BES also maintains ties with industry. Industry representatives participate in workshops and in reviewing research proposals, and in membership on advisory panels to the laboratories. They also use the specialized research facilities supported by BES. Through these and other mechanisms, the results of BES-sponsored research are continually made available to industry and the academic community.

Although the pursuit of research to broaden the technology base needed for identified energy technology options is important, even more important is the need for basic research unfettered by preconceived notions of which technologies will be important several decades from now, so that new, currently unidentified options may emerge. The following examples of research results in FY 1983-1984 that have enhanced energy alternatives or improved our understanding of energy-related phenomena are illustrative of the benefits to be gained from research in the basic energy sciences.

These accomplishments include:

o The preparation of simple, low-cost, yet very high efficiency solar cells from single crystal silicon. This method involves the novel application of two new technologies: ion implantation using a relatively inexpensive glow discharge source, and pulsed laser annealing.

o The development of a new thin film photoelectrode that can convert visible light to electricity or, in the photo-assisted electrolysis of water, can generate hydrogen. Many advances reported in photoelectrochemical energy conversion in the past two years have depended on ultraviolet light; this electrode can make use of the more abundant visible spectrum of the sun.

- The demonstration that the structure and surface hardness of ceramics can be modified and controlled by means of ion implantation to produce surface hardnesses that are greater or less than that of the original ceramic. The new technology involved gives us the ability to systematically alter the structure and properties of ceramic surfaces.

- The determination, based on research carried out under the Geosciences subprogram, that two recent volcanic eruptions, Mt. St. Helens in 1980 and El Chichon in 1982, have had and will have very different effects on climate. The effects of these eruptions have been sorted out through measurements of solar radiation reaching the earth during the past few years. The differences result from differing behavior of sulfur dioxide released by the eruptions in the formation of aerosol particles in the stratosphere.

- The measurement for the first time of fusion reaction rates using subatomic particles called mesons as reaction catalysts. The resulting reaction yield of neutrons is high and the application of the concept to provide high intensity neutron sources is possible.

- Progress in genetic engineering that makes it possible to transfer pieces of DNA carrying specific genes into host plants without causing the development of tumors in those plants, thus bringing the time closer when it should be possible to introduce desirable traits into plants to improve the species and, thus, the production of biomass which ultimately could be converted to energy.

Improvements in existing energy technologies and the development of new energy technologies invariably come from the application of just such new scientific knowledge. Given increasing international competition in science and technology, the need for a strengthened national basic research effort is clear. External blue ribbon advisory groups have repeatedly recommended that DOE increase its funding of basic energy research and have called for the Basic Energy Sciences program to be given a larger role in developing the needed technology base for the different energy supply and conservation options. Our FY 1985 budget request for Basic Energy Sciences is consistent with these recommendations.

An important aspect of Basic Energy Sciences research activities is the support of a number of national user research facilities. Recently, several facilities were brought on-line and each promises to open whole new areas of research possibilities. These facilities include: the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory; the Intense Pulsed Neutron Source (IPNS) at Argonne; the 1.5 MeV High Voltage Electron Microscope and the Atomic Resolution Microscope, located at Lawrence Berkeley Laboratory's National Center for Electron Microscopy; and the Combustion Research Facility (CRF) at Sandia Livermore. These facilities recently brought on-line together with existing ones (e.g., the Stanford Synchrotron

Laboratory), require significant increases in funding for their effective operation to assure their availability to meet the wide demand for experimental time by the research community. The facilities mentioned above are shown in figures 1-8. A complete list of BES user facilities is contained in Table 2. The Basic Energy Sciences program also is undertaking a new effort to provide needed access to supercomputers for ER-supported researchers. I will discuss that effort later in my testimony.

FY 1985 Budget Request

The FY 1985 BES budget was developed to focus on two principal objectives. The first is to maintain a strong core program -- this involves equipping, supporting and encouraging the scientists involved in our current program activities, and training new, younger scientists, to expand the forefront of knowledge in areas likely to be important to future energy technologies. The second objective is to provide for the operation of existing, unique facilities important to research in the U.S. while, at the same time, developing and constructing and providing for the future operation of needed new facilities. Additionally, in selected subprograms, opportunities for exploiting new, emerging areas, that have been identified as having great potential importance to energy, will be pursued.

The FY 1985 request for the BES program is $419.5 million. This budget which is composed of $348.3 million in Operating Expenses, $31.1 million in Capital Equipment and $40.1 million in Construction funds, maintains the needed continuity of the FY 1984 program (Table 3).

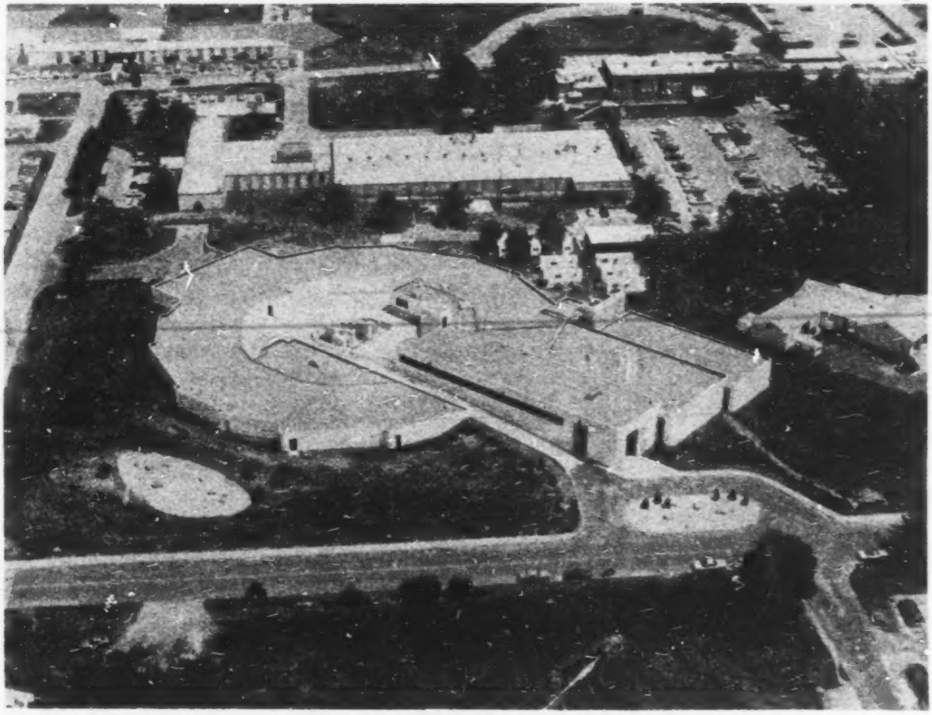

FIGURE 1. National Synchrotron Light Source—Brookhaven National Laboratory.

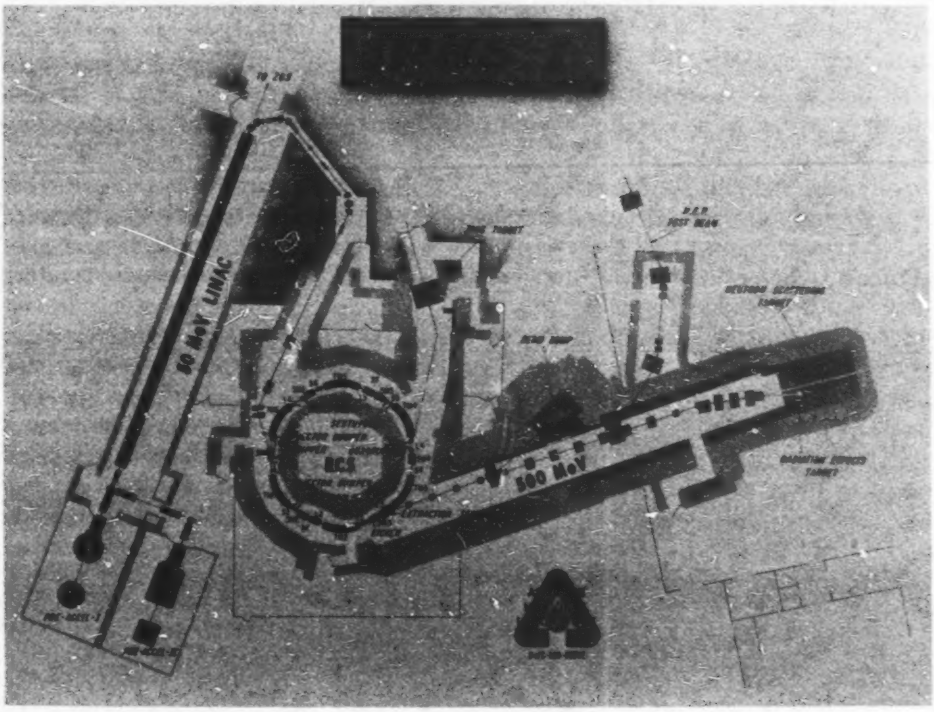
TO 203
50 MeV LINAC
RCS
EXTRACTION
BEAM DUMP
FAST BEAM
NEUTRON SCATTERING TARGET
500 MeV
RADIATION EFFECTS TARGET

FIGURE 2. Schematic of the Intense Pulsed Neutron Source—Argonne National Laboratory.

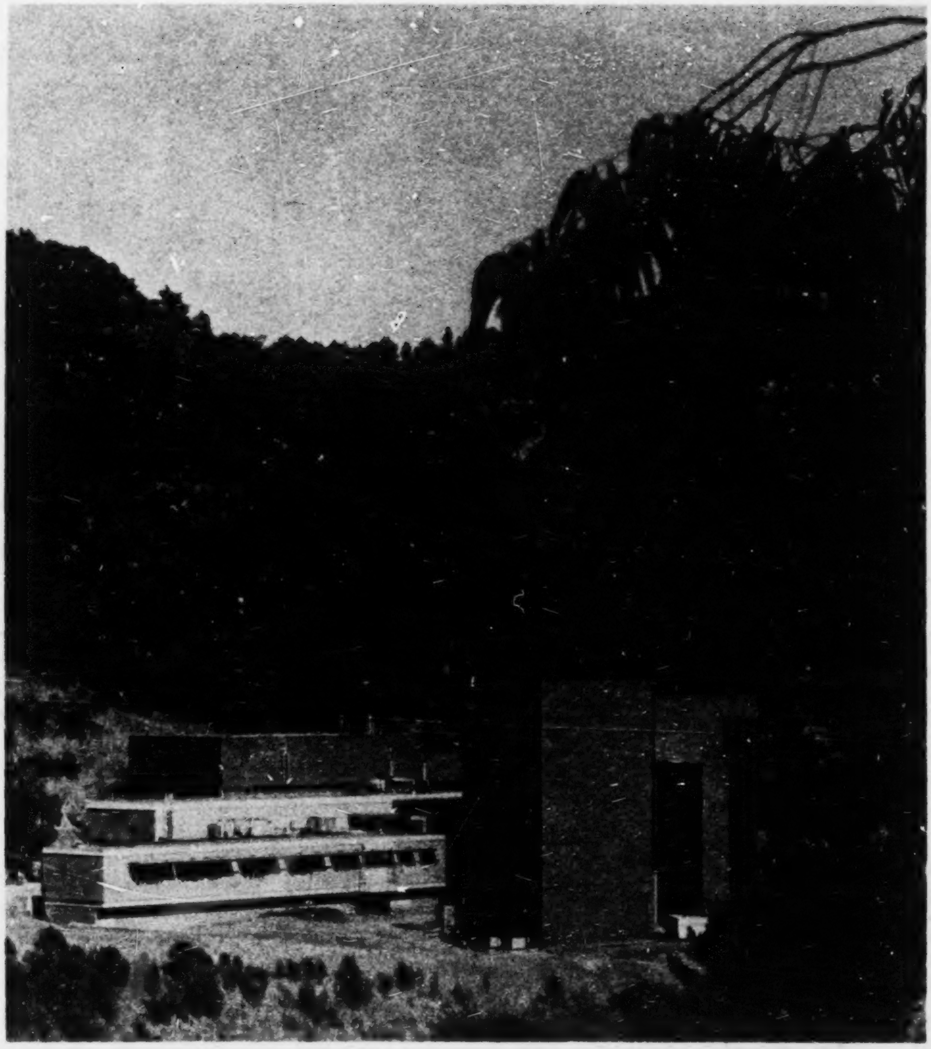

FIGURE 3. National Center for Electron Microscopy—Lawrence Berkeley Laboratory.

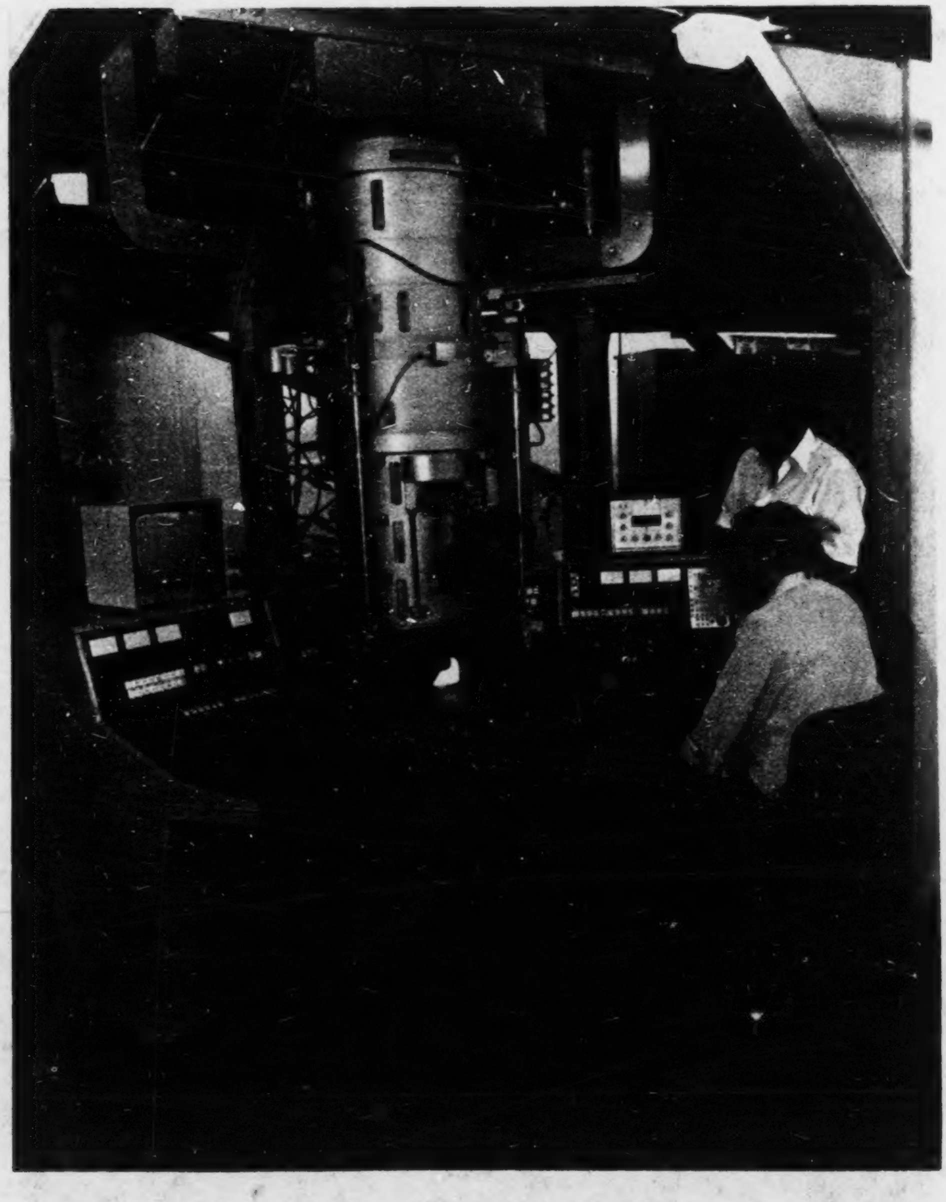

FIGURE 4. High Voltage Electron Microscope—National Center for Electron Microscopy (LBL).

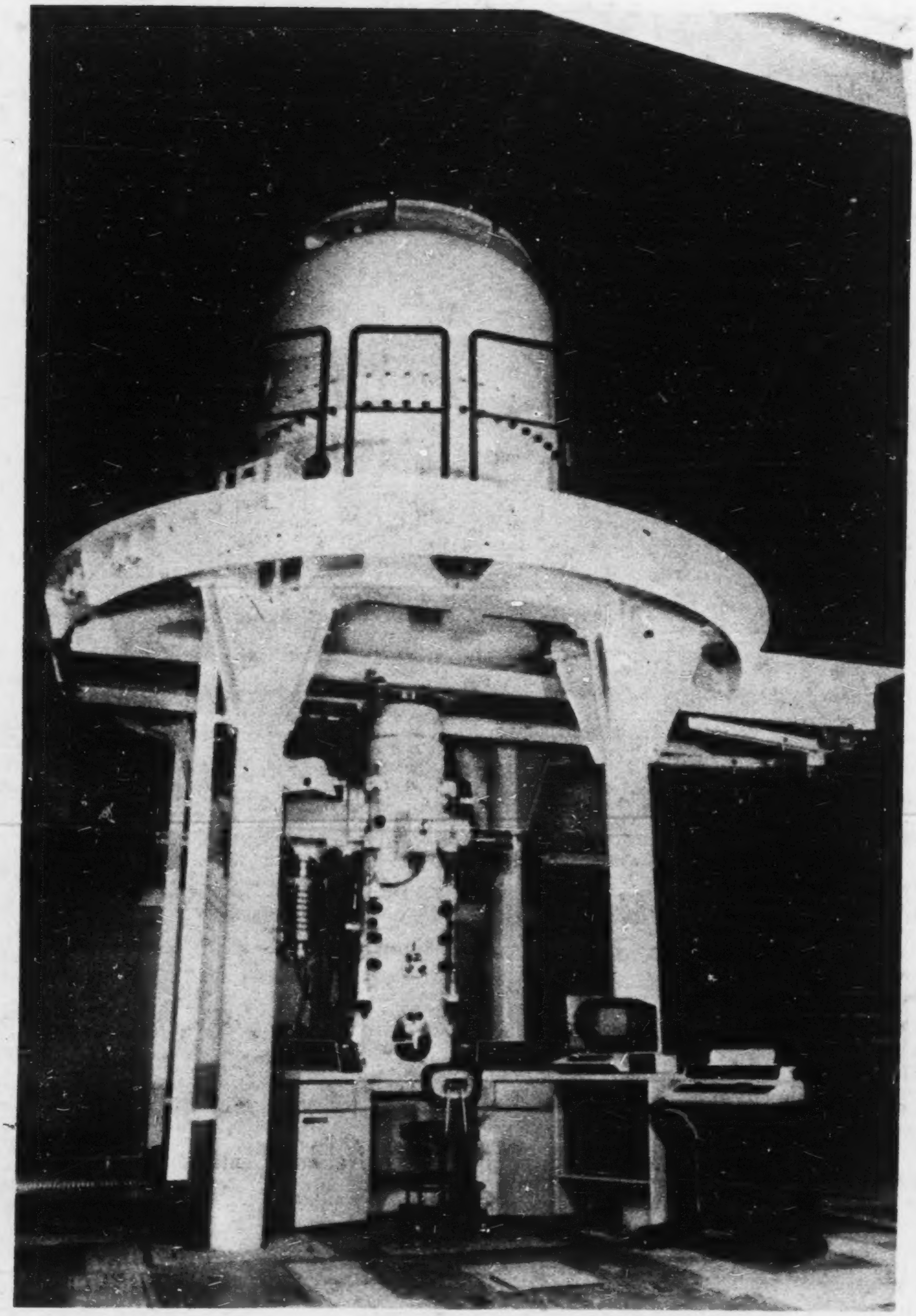

Figure 5. Atomic Resolution Microscope—National Center for Electron Microscopy (LBL).

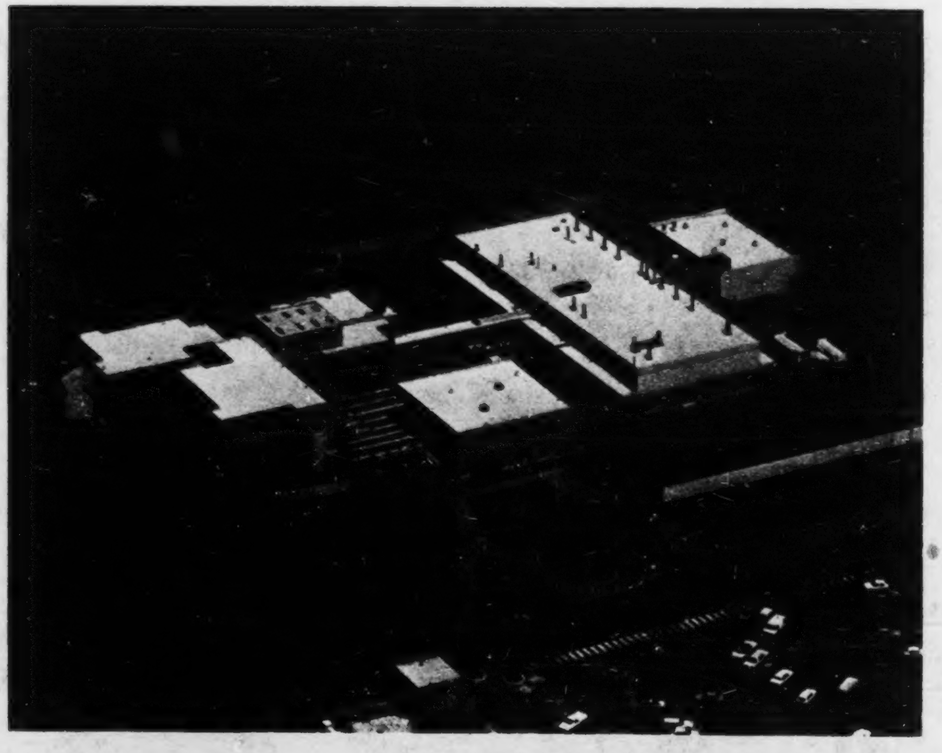

FIGURE 6. Combustion Research Facility—Sandia National Laboratories, Livermore.

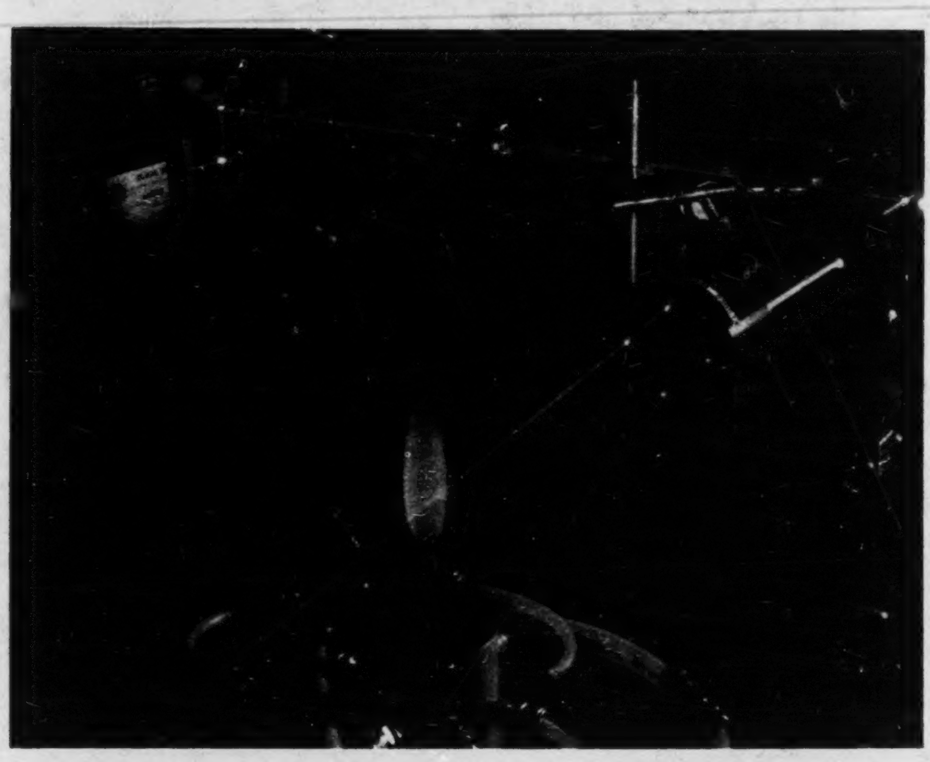

FIGURE 7. Flame experiment using laser at the Combustion Research Facility.

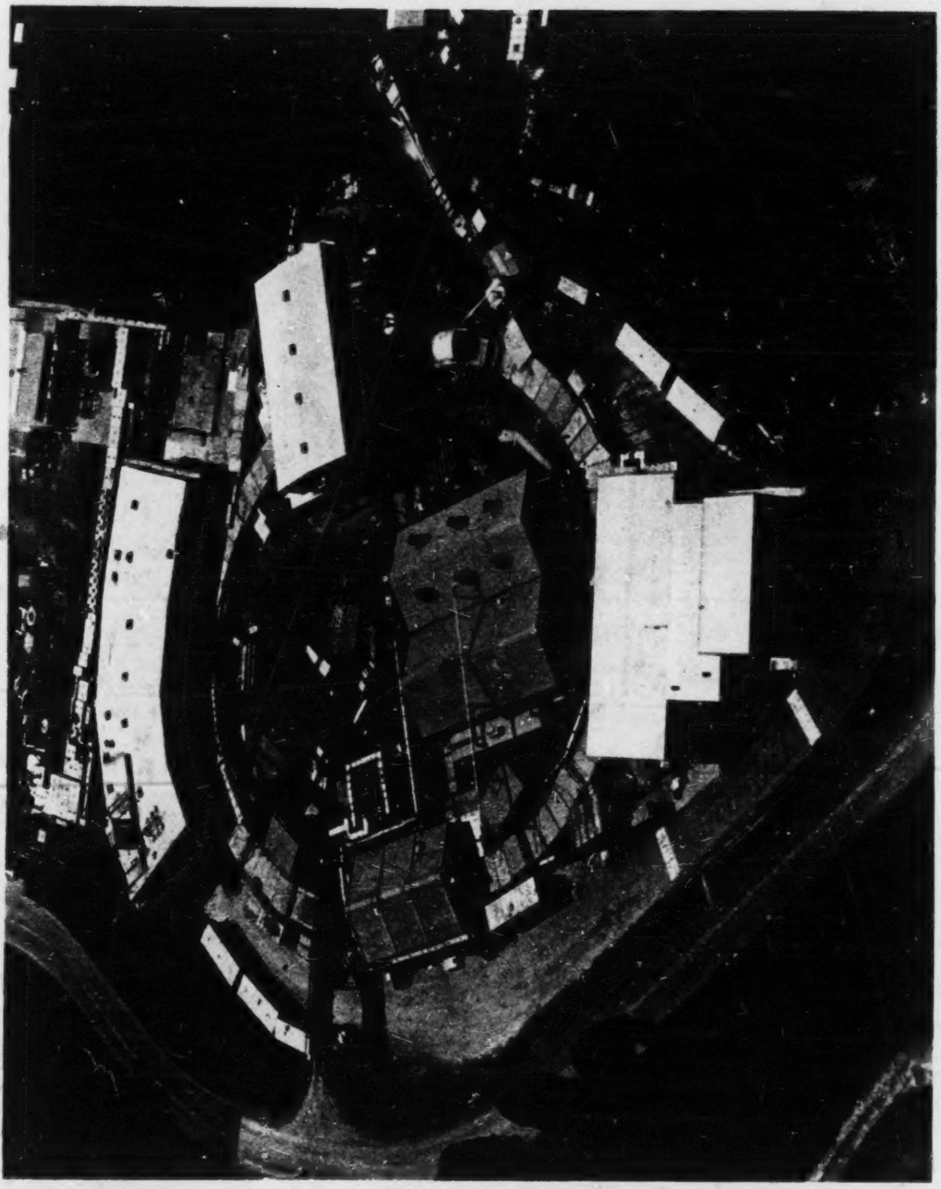

Figure 8. Stanford Synchrotron Radiation Laboratory—Stanford Linear Accelerator Center.

Table 2
Basic Energy Sciences Facilities

High Flux Beam Reactor (HFBR) - Brookhaven National Laboratory

National Synchrotron Light Source (NSLS) - Brookhaven National Laboratory

Intense Pulsed Neutron Source (IPNS) - Argonne National Laboratory

High Voltage Electron Microscope-Tandem Facility - Argonne National Laboratory

Oak Ridge Electron Linear Accelerator (ORELA) - Oak Ridge National Laboratory

High Flux Isotope Reactor (HFIR) - Oak Ridge National Laboratory

Combustion Research Facility (CRF) - Sandia National Laboratories, Livermore

National Center for Electron Microscopy - Lawrence Berkeley National Laboratory

Stanford Synchrotron Radiation Laboratory (SSRL) - Stanford University

Spallation Neutron Research Facility (SNR) - Los Alamos National Laboratory

Table 3
Basic Energy Sciences
Budget Authority
($ in millions)

	FY 1984 Estimate	FY 1985 Request
Operating Expenses		
Materials Sciences	$125.1	$141.5
Chemical Sciences	75.5	80.9
Nuclear Sciences	37.9	49.8
Applied Mathematical Sciences	14.6	28.2
Engineering and Geosciences	19.0	20.8
Advanced Energy Projects	9.1	10.8
Biological Energy Research	10.6	12.5
Program Direction	4.0	3.8
Subtotal	$295.8	$348.3
Capital Equipment	24.3	31.1
Construction	17.2	40.1
Total Basic Energy Sciences	$337.3	$419.5

The total Operating Expenses request for FY 1985 is $348.3 million, an increase of 18% over the corresponding FY 1984 level. Most of this increase is for cost of living increases for each BES subprogram, and to meet increasing costs of facility operations. A table (Table 4) has been attached which summarizes all of the increases for FY 1985.

Of the total BES request for Operating Expenses for FY 1985, almost 40% will be spent to operate or carry out research at the major BES facilities. These are used not only by the Department, but also by other Federal agencies, by industry and by university researchers. These facilities represent a national resource that is essential for a sound national research program. The budget request will ensure continued operation and access to these facilities in FY 1985. Equally important, we have provided additional funds in FY 1985 to operate the new state-of-the-art facilities that are only now becoming fully operational and that I mentioned earlier in my testimony.

The FY 1985 budget increase will also support promising new research that we believe will have a significant impact on energy. Two items in the request exemplify research areas with great potential. These are the materials sciences research initiative, which was started in 1984, and the budget request for the Applied Mathematical Sciences subprogram. Let me first discuss the materials initiative.

Table 4
Basic Energy Sciences
Explanation of Budget Changes from FY 1984 to FY 1985
($ in millions)

1984 Appropriation enacted	$337.3
Operating Changes	
Programmatic increases (described in detail below)	
Materials Sciences	+16.4
o Provides for increased funds for facility operations, reactor fuel element requirements and additional requirements associated with the advanced materials research initiative.	
Chemical Sciences	+5.4
o Provides increases for meeting facility commitments and reflects internal adjustments required to meet ongoing research commitments.	
Nuclear Sciences	+11.8
o Provides increases to meet commitments for the National Nuclear Data Program, an expansion to the Heavy Ion Fusion Program, and to meet facility commitments.	
Applied Mathematical Sciences	+13.6
o Provides increases for a significant expansion in basic research in scientific computing at national laboratories, universities and private research institutions. In addition, experimental computing capabilities are being established to support the exploration of new concepts in large scale scientific computing. Also, increase is provided for expanding access for Energy Research scientists to state-of-the-art computing capability.	

Other Operating Changes	+5.3
o Provides increases in Engineering and Geosciences, Advanced Energy Projects, Biological Energy Research, and Program Direction necessary for expansion of those research activities holding the greatest promise.	
Subtotal Operating Changes	52.5
Capital Equipment Changes	
o Programmatic increase in each of the subprograms will be provided to meet facility requirements, to support the recently assigned responsibility for General Purpose Equipment at Argonne National Laboratory, and to support new requirements in areas of increasing research.	+6.8
Subtotal Capital Equipment Changes	6.8
Construction Changes	
o Programmatic increases for General Plant Projects (Argonne National Laboratory, Ames Laboratory, Notre Dame University, and Stanford University); Accelerator Improvement Projects; Kansas State Univeristy Ion Collision Physics Facility; National Synchrotron Light Source; Center for Advanced Materials and Stanford Synchrotron Radiation Laboratory Enhancement.	+22.9
Subtotal	22.9
1985 budget request	$419.5*

*The FY 1985 budget request reflects $3.0 million for savings resulting from management initiatives related to administrative processes.

The United States' economic health and national security require the maintenance of a commanding lead in high technology and reduced vulnerability to critical and strategic imported materials. In response to this challenge, an advanced materials research initiative was first proposed in FY 1984. The current budget initiative consists of a Center for Advanced Materials (CAM) at Lawrence Berkeley Laboratory (LBL), improvements at the Stanford Synchrotron Radiation Laboratory and an expansion of activities at the National Synchrotron Light Source at the Brookhaven National Laboratory.

Planned activities in FY 1984 and the FY 1985 budget request are consistent with the recommendations of an ad hoc panel composed of leaders from industry, academia and the national laboratories. This panel was established in April 1983 to review the initial proposal for a center for advanced materials. Those recommendations were to continue the initiative, but to decouple the synchrotron radiation facilities from the advanced materials research and treat them separately. The panel made a number of constructive recommendations which have been factored into this year's request. A new National Academy of Sciences study of the requirements for additional major facilities currently is underway. Decisions to proceed further with construction of major new facilities will await the results of that study.

The ongoing advanced materials research is being organized to provide maximum benefit to the Nation. Industry will participate in the design of the CAM program to assure that the research addresses America's high-technology needs. For example an advisory board composed of scientific leaders from industry, universities, and Federal laboratories will advise the Director of LBL, home of the Center for Advanced Materials, on the scientific program directions for CAM. An Industrial Fellows program has been established to provide joint LBL-industrial participation in basic research studies of mutual interest to LBL and the scientists' parent companies. An initial workshop on general concerns regarding industrial participation was held in 1983 where issues and follow-on activities were agreed upon. Four CAM workshops for the initial research areas have been held with strong industry participation.

The second expanded research activity I would like to highlight is in our Applied Mathematical Sciences subprogram for which we have requested $29.7 million in FY 1985. Supercomputers are playing an increasingly important role in many of the Department of Energy's programs. Every generation of large scientific computers has had a significant positive impact on the ability of the DOE laboratories to meet their mission goals. Each new machine has improved the laboratories' abilities to more accurately model complex physical phenomena, thus improving their productive capability and reducing the number of expensive tests now required.

Evidence of this improved capability has already been seen in the design and testing of nuclear weapons and more recently in magnetic fusion research. As they have become available, DOE programs in fundamental physical sciences are just beginning to use supercomputers as "experimental" devices for theoretical calculations. The need for large scale scientific computers is emerging in high energy physics, condensed matter research, and chemical and biological theory. Calculations of subatomic particle confinement, critical phenomena in alloy solidification and superconductors, thermophysical properties of chemical mixtures, and properties of long-chain polymers are providing insight into the basic properties of matter.

The Applied Mathematical Sciences subprogram consists of two activities. The first (Supercomputing Research) is aimed at funding research in mathematical and computational sciences that is critical to the use and development of future supercomputer systems. The second activity (Energy Science Advanced Computation) will provide network access to large-scale scientific computing required by several Departmental programs and to the basic research activities funded by the Office of Energy Research in universities, national laboratories and industry.

The goal of the Supercomputing Research activity is to advance our understanding of the fundamental concepts of mathematics, statistics, and computer science underlying complex mathematical models of the key physical processes in energy systems. Much of the scientific research and development effort throughout DOE programs is focused directly on analytical and numerical modeling of these physical processes. Basic research in the relationships among the mathematical formulation of scientific and engineering problems, the creation of algorithms for solving these problems and the architectures of parallel computers designed to implement these algorithms is vital for developing future energy systems.

The Energy Science Advanced Computation activity is aimed at meeting the immediate needs for supercomputer access by the Department of Energy's High Energy and Nuclear Physics, Biological and Environmental Research, and Basic Energy Sciences programs. The substantial contribution to solving the national problem of providing access to supercomputers for energy researchers will help to ensure that the U.S. maintains its lead in computational sciences related to supercomputer technology.

Capital Equipment

The Capital Equipment request for FY 1985 is $31.1 million, an increase of $6.8 million over FY 1984. This level of funding is necessary to meet ongoing research requirements, additional commitments associated with the newer facilities, and additional equipment for those selected areas of promising research. Examples of equipment to be purchased include an analytical electron microscope at Los Alamos National Laboratory, neutron scattering equipment, synchrotron radiation equipment and electron microscopy equipment. Two significant items in our request for FY 1985 deserve special note. The first, is a $1.5 million request for peripheral computer equipment which is an integral part of the Applied Mathematical Sciences expanded effort. Secondly, the BES request includes $2.0 million for the General Purpose Equipment needs at the Argonne National Laboratory site. Beginning in FY 1985, this responsibility has been transferred to BES from the Office of the Assistant Secretary for Nuclear Energy.

Construction

Table 5 details the Construction request for FY 1985. Three of the projects are associated with our materials initiative. Another new project will expand our atomic physics capability through the construction of an ion collision physics facility. In conjunction with existing capabilities, this facility will allow researchers to study the atomic physics of a range of ions at energies unmatched in the world. The project will be located at Kansas State University and will be jointly funded by DOE and the University, with the University providing the conventional construction necessary to house the new facility. The remaining construction funds are requested for General Plant Projects (GPP) and Accelerator Improvement Project (AIP) requirements. The request in FY 1985 includes a significant increase in GPP funds as a result of the BES program assuming GPP funding responsibility for the Argonne National Laboratory. Previously this funding was provided by the Assistant Secretary for Nuclear Energy. This item accounts for $5.0 million of the $5.8 million GPP request in FY 1985.

Table 5
Basic Energy Sciences
Budget Authority
($ in millions)

Construction

	Prior Years	FY 1985 Request	TEC	Completion Date
Accelerator Improvement Projects (85-ER-401)	$ 1.3	$ 2.4	$ 2.4	FY 1986
General Plant Projects (85-ER-400)	.4	5.8	5.8	FY 1986
NSLS Beam Line & Support, BNL (84-ER-111)	2.5	10.0	19.7	FY 1986
Center for Advanced Materials, LBL (84-ER-112)	1.8	10.8	40.2	FY 1988
Stanford Synchrotron Radiation Laboratory Enhancement (85-ER-402)	1.2	9.1	12.9	FY 1986
Kansas State University Ion Collision Physics Facility (85-ER-403)		2.0	3.4	FY 1987
Total		$40.1		

This completes my summary of the BES program. I would now like to discuss the several ER outlay programs that are related to my statutory responsibilities to advise the Secretary on DOE energy R&D programs, the non-weapons multiprogram laboratories and the education and training of scientists and engineers.

ADVISORY AND ASSESSMENT ACTIVITIES

Within the Office of Energy Research, the Office of Field Operations Management (FOM) and the Office of Program Analysis (OPA) support the Director's advisory responsibilities. The Office of Field Operations Management provides support with regard to oversight of the laboratories and energy-related manpower development and training activities. This Office has developed several management tools used by the Department in administering its laboratories and R&D facilities across the country. It also continues to manage the University Research Support, the University Research Instrumentation and the Multiprogram General Purpose Facilities programs, all of which I will discuss shortly. The Office of Program Analysis, on the other hand, provides independent and objective program analyses and technical assessments under the Energy Research Analyses program. The FY 1985 budget request for these four programs is shown in Table 6.

Table 6
Energy Research Analyses, University Research Support, University Research Instrumentation, Multiprogram General Purpose Facilities
Budget Authority
($ in millions)

	FY 1984 Estimate	FY 1985 Request
Operating Expenses		
Energy Research Analyses	$ 2.9	$ 3.0
University Research Support	5.5	9.2
University Research Instrumentation	4.0	6.0
Construction		
Multiprogram General Purpose Facilities	42.1	39.0

ENERGY RESEARCH ANALYSES

With an FY 1985 budget request of $3.0 million, the Energy Research Analyses program provides the Department with a capability for independent analyses of its technical needs and opportunities. It is carried out by the Office of Energy Research (ER) through studies, workshops, panels, and other mechanisms that allow the Department to make use of the best talent available from the industrial and academic sectors as well as the national laboratories. The specific functions of this program include assessing DOE's long range technology base and ongoing R&D programs, providing coordination and direction for interagency activities such as acid rain, coordinating resolution of major technical issues and research policy developments, and providing support to DOE advisory groups such as the Energy Research Advisory Board.

Recent accomplishments in the area of technical assessments included completion of two major program assessments, one of university and laboratory research projects in the Office of Fossil Energy's Enhanced Gas and Oil Recovery Program and the other of the accomplishments of ER's Biological and Environmental Research (BER) program. The latter assessment documented tangible contributions to the public made by the BER program. A narrative of these accomplishments is now available.

Assessments of research needs and priorities regarding photovoltaic cells and the solar thermal and geothermal programs were also completed. These independent reviews by outstanding researchers provided peer guidance on the most fruitful directions for future DOE research. An assessment was made of solar and building control research projects supported by DOE at the National Bureau of Standards. This work was found to be of high quality and appropriate for support by the public sector. Finally, an assessment of the need to continue the DOE High Altitude Sampling Program was completed.

OPA continued to represent DOE on the Interagency Task Force on Acid Precipitation and to coordinate the DOE acid precipitation research program with other Federal agencies. In FY 1983, DOE and the Environmental Protection Agency entered into a Memorandum of Understanding (MOU) initiated by OPA. The MOU formalized the joint assessment efforts of the two agencies and established the Acid Deposition Assessment Staff to which OPA continues to provide manpower and financial support. In addition, OPA conducted extensive technical contributions to documents used by those who formulate the Administration's acid rain policy.

The FY 1985 budget request would provide up to four technology assessments depending on their complexity and depth and up to four program assessments. Technical coordination and guidance will continue in the areas of acid rain and civil remote land sensing; liaison responsibilities will continue with the International Energy Agency to maintain annual reviews of energy R&D

priorities, programs and technology base. The program will also provide independent peer review of technical or research subjects as requested by principal Secretarial Offices or the Director of Energy Research, and will continue to support the Energy Research Advisory Board.

UNIVERSITY RESEARCH SUPPORT

The University Research Support Program (URS) provides a budget and management focus for a small number of specialized research and manpower development activities which help strengthen the capabilities of both universities and the Department's laboratories to carry out longer range scientific and technical research. Through these interrelated efforts, the Department is working to:

- o Maintain and strengthen university-based energy research and manpower development efforts in selected high priority energy research fields.
- o Utilize the unique resources of the national laboratories (equipment, instrumentation, and personnel) to assist university faculty and students to carry out advanced research and related training.

- o Increase the number of students including women and minorities pursuing professional level degrees in energy-related science or engineering.
- o Enhance the quality of the scientific/technical workforce in the Department's national laboratories.

The URS program, with an FY 1985 budget request of $9.2 million in Operating Expenses, consists of two major subprograms (Table 7). The first subprogram, University/National Laboratory Cooperative Research, is directed at strengthening the capabilities of both universities and national laboratories as major energy research performers in the conduct of long range energy research. Many of the activities supported within this subprogram involve joint efforts between university and laboratory-based researchers. With a FY 1985 budget request of $8.4 million, this subprogram supports both University Laboratory Cooperative Research and the University Reactor Fuel Assistance. This latter activity is aimed at ensuring that a continuing fuel supply is available for operation of university research reactors.

We are requesting a significant increase ($3.0 million) for the University Laboratory Cooperative Research activity. This program serves as an essential bridge, and will strengthen the ties, between the laboratory and university communities. Laboratories are important complementary resources

Table 7
University Research Support
Budget Authority
($ in millions)

	FY 1984 Estimate	FY 1985 Request
Operating Expenses		
University/National Laboratory Cooperative Research		
University Laboratory Cooperative Research	$ 3.5	$ 6.5
University Reactor Fuel Assistance	1.5	1.9
Subtotal	$ 5.0	$ 8.4
Energy Manpower Development		
Energy Manpower Assessment	$ 0.3	$ 0.5
Energy Education & Training	0.2	0.3
Subtotal	$ 0.5	$ 0.8
Total University Research Support	$ 5.5	$ 9.2

in preparing students for future research careers. This budget request will allow us to double the number of undergraduate students supported in summer research programs. It also will allow us to develop additional cooperative research programs involving university faculty and graduate students and laboratory scientists.

The second subprogram, Energy Manpower Development, with a FY 1985 budget request of $0.8 million in Operating Expenses, combines two manpower-oriented activities. The Manpower Assessment activity conducts assessments and analyses of the supply and demand of manpower for both current and future energy R&D programs; and Energy Education and Training supports activities directed at encouraging secondary school students to pursue energy-related science and engineering programs at the college level.

The FY 1985 budget request of $9.2 million in Operating Expenses will allow these programs together to:

- Support approximately 3000 student and faculty research participation appointments and special training activities at the Department's national laboratories and major contractor facilities,

- Refuel up to six university research/training reactors and support approximately 18 reactor sharing projects,

- Update manpower assessments for future professional level manpower requirements (e.g., scientists/engineers) for Departmental research programs,
- Support cooperative projects with universities, industry and the Department's national laboratories through the Prefreshman Engineering Program designed to encourage secondary school students to pursue energy-related engineering and science programs during their college careers, and
- Support 6-8 high school science and math teacher institutes in computer science and energy-related subjects at the DOE national laboratories.

UNIVERSITY RESEARCH INSTRUMENTATION

The continued improvement of energy technologies depends on the development of new knowledge and concepts that can be applied to energy-related materials and processes. The research that leads to this new knowledge requires advanced, state-of-the-art equipment.

The types of instruments required for advanced energy research include such equipment as plasma emission spectrometers which will detect and identify materials at the parts per billion level, a variety of scanning microscopes which can be used to obtain greater understanding of surface states and features, and hydrothermal equipment which enables one to simulate the temperatures and pressures which are found deep within the earth and in ocean depths. These and related instruments are very expensive, generally on the order of several hundred thousand dollars, and thus beyond the means of nearly all research universities to finance directly.

In recent years the Department has attempted to help universities obtain access to these and similar sophisticated research instruments by (1) making the equipment at its national laboratories available to university researchers, (2) establishing unique user-oriented research facilities such as the Combustion Research Facility at the Sandia Laboratory at Livermore and (3) providing some funds for the less expensive research tools required in conjunction with its research projects.

None of these programs, however, meets the needs of university scientists for continuous availability of the type of equipment which is provided through this program. This continuous and direct access to state-of-the-art instrumentation often determines whether scientists can produce frontier-level results.

DOE's University Research Instrumentation program, with an FY 1985 budget request of $6.0 million in Operating Expenses, will focus on those university groups that have demonstrated expertise in one or more of a small number of energy-related topics which are of special concern in the Department's long-range research efforts. Among the research topics likely to be of concern in FY 1985 are combustion, bioconversion related to energy, nuclear waste isolation systems, catalysis, advanced materials science and engineering, and the transport of energy-related pollutants. It is estimated that the $6.0 million requested will enable the Department to assist about 10-20 institutions to obtain the expensive (i.e., over $100,000) specialized instrumentation required.

The program will continue to be coordinated, including both proposal review and awards, with similar programs in the other Federal agencies such as DOD and NSF. The close coordination ensures that each agency's program complements and reinforces the research efforts of all the agencies and makes each program more cost effective.

MULTIPROGRAM GENERAL PURPOSE FACILITIES

The FY 1985 Construction request for the Multiprogram General Purpose Facilities (MGPF) program is $39.0 million (Table 8). The goal of this program, which is managed for the Department by the Office of Energy

Table 8
Multiprogram General Purpose Facilities
Budget Authority
($ in millions)
FY 1985 Proposed Projects

	FY 1985 Request
Construction	
Central Chilled Water Facility, BNL (85-R-701)	$ 3.5
Replace Laboratory Roofs, ANL (85-R-702)	3.5
Electrical Distribution System Restoration, ORNL (85-R-703)	1.1
Rehabilitate Underground Steam System, ANL (85-R-704)	3.0
Medical Facility Replacement, LLNL (85-R-706)	1.6
Replace Site Fire Alarm System, RL (85-R-707)	1.3
Establish a Central Chilled Water Plant, ANL (85-R-709)	1.0
Upgrade Environmental Monitoring, ORNL (85-R-711)	1.0
Modify Central Chilled Water Plant, ORNL (85-R-712)	1.0
Prior Year ongoing projects*	22.0
Total	$39.0**

*See Table 9 for additional detail on prior year ongoing projects.
**FY 1984 estimate for MGPF program is $42.1 million.

Table 9
Multiprogram General Purpose Facilities
Budget Authority
($ in millions)

	FY 1985 Request
Construction (ongoing projects)	
Security Facility, ANL (82-E-302)	$1.1
Rehabilitate Power Systems, INEL, LLNL, RL,ORNL (83-E-308)	2.8
Electronics Facility. ANL (83-E-309)	3.2
Utility Replacement & Upgrade, BNL (83-E-310)	3.2
Rehabilitate Old Town Utilities, LBL (84-ER-101)	3.8
Cooling Water Facility Rest., ORNL (84-ER-102)	3.4
Road Repair, LBL, INEL, RL, ANL (84-ER-103)	4.5
Subtotal Ongoing	$22.0

Research, is to rehabilitate and replace multiprogram general support facilities that are essential to continued operations of the Department's multiprogram laboratory sites. These support facilities include site utilities and support buildings such as laboratories, office buildings and warehouses, roads and railroads, which represent a multibillion dollar government investment.

Through continued use and aging, support facilities deteriorate to a point where they are no longer capable of performing their intended functions and must be rehabilitated or replaced. The MGPF program systematically reduces the backlog of deficiencies of these support facilities. It reflects an appropriate Federal responsibility for management of the Government's real property, and we plan to continue the program as a necessary cost of doing business as long as the multiprogram laboratory facilities are used to perform research and development functions for the Department.

The FY 1985 budget request would continue construction on several projects begun in prior years, including rehabilitation of the Old Town area utilities at LBL, the upgrade of the cooling water facility at ORNL and improvements of roads at various laboratories. New projects proposed for FY 1985 would include rehabilitation or replacement of such facilities as an electrical distribution system (ORNL), an underground steam system (ANL), laboratory roofs (ANL), chilled water facilities (BNL, ORNL, ANL), medical facilities (LLNL), a fire alarm system (RL), and an environmental monitoring system (ORNL).

ADVISORY AND OVERSIGHT PROGRAM DIRECTION AND POLICY AND MANAGEMENT

The FY 1985 budget request for Advisory and Oversight Program Direction is $2.9 million. These funds are required to provide for the salaries, benefits, travel and other expenses associated with 44 full-time equivalents. This FY 1985 request will provide the staffing resources required by the Director of Energy Research to carry out his responsibilities under legislation (P.L. 95-91) and those mandated by the Secretary in areas beyond the scope of other ongoing Energy Research programs.

The FY 1985 budget request for Policy and Management is $0.5 million. These funds are required to provide for the salaries and related expenses associated with 8 full-time equivalents in the Office of the Director of Energy Research.

Mr. Chairman, this concludes by testimony. I would be pleased to answer any questions at this time.

Mr. FUQUA. Thank you very much, Dr. Trivelpiece. It is my understanding Mr. Winn has a statement he wishes to insert in the record following my opening statement.

[The opening statement of Mr. Winn follows:]

STATEMENT OF HON. LARRY WINN, JR., ENERGY DEVELOPMENT AND APPLICATIONS SUBCOMMITTEE

Mr. Chairman, thank you for this opportunity to welcome Dr. Trivelpiece back today. His testimony on the High Energy Physics and Nuclear Energy Programs was very helpful and I am certain our discussion on the basic energy sciences and asset management will also be beneficial.

The Basic Energy Sciences program request for fiscal year 1985 of $420 million exceeds last year's appropriation of $337 million by almost 25 percent. That is an impressive increase in these times of budget strain. It is interesting that DOE proposes to administer this substantial increase at a lower program direction cost. What managerial breakthrough has occurred? It is certainly welcome.

These programs are a step nearer to application than yesterday's discussion. So, one can expect increasing industry involvement. Yet a recent Energy Research Advisory Board report on materials research mentioned industry and technology transfer only in the last portion of the text.

We continually hear our colleges and universities claim that they participate to a very small extent in some DOE programs. Maybe that is not true of the Basic Energy Sciences programs. Or is it?

All these basic research programs add asset upon asset, at an escalating rate and we realize that equipment becomes increasingly expensive. But what of the maintenance required? What percentage of total funding is used to maintain the facilities we have already purchased? Are present assets being sacrificed to buy new initiatives? Are care and preservation growing at the same rate as programs?

We are aware that DOE receives many proposals each year which require review, comparison, priorities and scheduling. There is not enough money to fund all the worthy projects at once, so prudent evaluation is necessary, and appears to be practiced. However, two projects last year by-passed that review process through partisan political footwork and DOE succumbed to the pressure, deciding to review only the projects, not their justification. Understandably, the science community has expressed deep concern. I recently co-sponsored a resolution calling for a return to peer review, and many Members share my feelings in this matter.

Mr. Chairman, I trust we will get response on these observations and questions which will be beneficial to the Committee this year. Thank you.

Mr. FUQUA. The long concern of the committee has been, since several years back, a lack of coordination of facilities, particularly the maintenance and upkeep of facilities, where they would be deferred for other years and so forth. It was never coordinated from the departmental headquarters; a real coordinated review of federally owned facilities operated out in different places. Has that changed? This may not be in your category, although I guess some of it falls within your responsibility at some of the national laboratories. There was a great deal of concern that there was not any coordination. We attempted to try to establish something within the top echelon of the Department of Energy that would coordinate that.

It should be somebody who knows something about facilities, not necessarily a physicist or somebody who was familiar with that field. They should know if the building needed painting, or when it needed painting, or when did the air-conditioner or heating system need certain repairs. They would know that it was on a scheduled basis and not haphazard and maybe squeezing researchers out. I do not know, but we do have a considerable investment in those facilities, and they should be utilized in the most efficient method that we can. I was wondering what has happened recently about that.

Dr. TRIVELPIECE. I would not be so foolish as to say we solved the problem. I would, however, be bold enough to say that we have paid special attention to it in the Department, and as part of my responsibilities for the health and well-being of the laboratories, the statutory aspect of the Energy Research Director's job, I am involved with the Secretary and with one of his special assistants, Mr. Gjelde, in an activity which is called the Laboratory Management Council. That consists of the secretarial officers in the Department who have responsibilities for the program activities, and we review these things now. This was only done this last year at Secretary Hodel's request to establish such a council.

[The material referred to follows:]

LABORATORY MANAGEMENT COUNCIL

I would like to insert for the record the procedures by which the Laboratory Management Council operates.

The Laboratory Management Council, which supersedes the Field and Laboratory Coordination Council, was established by the Secretary on September 22, 1983. The Council consists of the programmatic officials responsible for research and development activities taking place at the laboratories which are under the Department's cognizance. It reviews significant issues and policy questions pertaining to the utilization and management of these laboratories.

Specifically, the Chairperson is the Special Assistant to the Secretary and includes as its members the Director of Energy Research, Assistant Secretaries for Defense Programs, Nuclear Energy, Fossil Energy, Conservation and Renewable Energy and Management and Administration. Additional Headquarters officials are invited on case-by-case basis depending on agenda items.

There is no funding for the Council.

Mr. FUQUA. Could you provide us for the record the procedures by which that operates so we can take a look at that? Before this administration came in, we were expressing astonishment at some of the things that were going on at some of the laboratories. Let me commend you for that. If you could, we would like to take a look at that and help in any way we can.

Dr. **Trivelpiece**. We did give special attention to GPP and GPE and prepared some cross-tables to look at the different laboratories and how these funds were at them, as well as the historical record, as well as the circumstances that had occurred, where some program officials had chosen to sacrifice facilities at the expense of programs. I understand the dilemma in which they found themselves; it is a very human dilemma. But this is a corporate responsibility, and it needs to be addressed at the corporate level within the Department. We believe we have both organized it and raised it to the proper corporate level, and it remains to be seen whether or not we are eventually successful in providing the proper level of support for these kinds of things.

Mr. **Fuqua**. If we do not provide it in some fashion in a sound management basis, then at the end we find ourselves with inadequate facilities, incapable of carrying out the missions that they should, and then we have to spend a lot of money which, in turn, squeezes out a lot of research. It is a kind of a Catch-22 situation but one, I think, sound management would require that there be a periodic review of the maintenance and upkeep of our facilities.

Dr. **Trivelpiece**. We are not the only institution that suffers this particular problem, from the water system in New York City to the roads here in the District of Columbia to our freeway system. I think it is a serious national problem of how we are eating our capital in many areas and not paying proper attention to the maintenance of it, which I think in the long run turns out to be foolish economy.

Mr. **Fuqua**. Maybe you could do some research in the materials area. In addition to hips, maybe potholes.

Dr. **Trivelpiece**. I would be delighted. Unfortunately it seems that there is a water-soluble asphalt which can develop in this Nation.

Mr. **Fuqua**. In the basic energy science program, there is included in the budget about $5 million for the GPP and $2 million in the GPE funding for Argonne Laboratory. They have been funded out of the nuclear programs in recent years. Why has that been changed?

Dr. **Trivelpiece**. There is a principle of having the program that has the largest activity at a given national laboratory be the landlord with respect to those kinds of funds. It would be, from an accounting point of view, a nightmare to try to allocate a portion of that maintenance activity to all the programs, so it is put in one program as a matter of practice. The nuclear programs have done just what I said. They did not maintain this at the level that was thought to be appropriate for the Department, and that responsibility was transferred to Energy Research. And that is why it appears in the budget to be carried in one of the elements of the BES program. It could be allocated to all the other programs that are at Argonne, but it is just a matter of practice, administrative practice in the Department, to assign it to one element. We think that is a sound approach. So it appears here where you can look at it as a total entity, rather than having to discover where it is located in all the other programs that the Department has there.

Mr. **Fuqua**. In the budget request for transportation energy conservation program, there is about a $5.5 million addition for operating expenses, about a 200-percent increase. It is for advanced materials development subprogram, and the energy conservation and utilization technologies program has requested an additional $3.7 million, an increase of about 160 percent, for the material science project. I guess the question is, How do these activities supplement or complement or duplicate any other of the basic energy science program requests?

Dr. **Trivelpiece**. I am not sure which elements you are talking about.

Mr. **Fuqua**. In the BES materials research program, are these duplicating, complementing, or additional funds that you are requesting in the transportation energy conservation program of $5.5 million and in the energy conservation and utilization technologies program there is an increase of $3.7 million. Are they duplicating any of the other work that is going on in the BES?

Dr. **Trivelpiece**. I am sorry, I do not know the answer to that. Perhaps Dr. Kropschot can respond to your question.

Dr. **Kropschot**. The two programs, the one in conservation is what we call applied ceramics for engines. We have coordinated between basic energy sciences and that program to have the programs meshed. Our programs in the fundamentals of ceramics and their program of the applied nature. We have an upcoming workshop which will involve their program people, our program people, the industry that will be using the ceramics. This is a coordination effort, a long-term program planning effort, and a developmental activity for ceramics to span the areas from the very basic work that we do to the applied work that conservation does to what the industry needs eventually. The meshing of those programs is worked out fairly carefully on our part is a program that needs substantial additional support.

Mr. **Fuqua**. This would be in the applied area then that the additional funds are being requested?

Dr. **Kropschot**. Yes.

Mr. **Fuqua**. Is it other than just ceramics? Other materials?

Dr. **Kropschot**. I believe I am correct in saying yes, it is.

Mr. **Fuqua**. That would be for automobile engines and so forth?

Dr. **Kropschot**. Yes. On our end, the basic part of the materials that go in, the characterization of materials, and the material research effort is developed as part of our center for advanced materials, as well as other parts of the research program conducted in other laboratories.

Mr. **Fuqua**. Dr. Trivelpiece, there was about $54 million requested from OMB for the Energy Science Research Computation Initiative. It appears that there are not any funds in the applied mathematical sciences program that were included in the Energy Science Research Computation Initiative.

Dr. **Trivelpiece**. There is approximately a total of $30 million, which is in the budget at the moment. Of that, approximately $16 million is the original applied math program. The remaining portion, approximately $14 million, is for the supercomputer activities, and that involves two elements of approximately equal amounts. One is to provide additional access, and the other is to begin some research on parallel processing and related activities.

Mr. **Fuqua**. Where does the other $20 million come from? There is $54 million.

Dr. **Trivelpiece**. You have to ask OMB. It is not part of the President's budget.

Mr. **Fuqua**. One of the justifications was that a state-of-the-art supercomputer be leased to satisfy the computational requirements of the energy science program. What type of computer are you planning to lease, and where will it be located?

Dr. **Trivelpiece**. The plan at the moment is to have a class 6 system, which is a Cray or a Cyber 205, and to locate it at the Lawrence Livermore Laboratory as part of the fusion computer center and take advantage of the preexisting network, communications network, that exists for the fusion program and allow additional users in high-energy physics, nuclear physics, and the life sciences and basic energy sciences to take advantage of it.

As I said in my earlier testimony on supercomputers, part of our plan is to provide access to ER contractors as rapidly as possible with what we have available, and we think that is the most rapid way to accomplish that objective.

Mr. **Fuqua**. Would that include university and other DOE laboratories and industrial researchers?

Dr. **Trivelpiece**. As long as they are DOE contractors, then yes, it is possible. We are not in business to compete with private vendors who sell computer time. We cannot provide it to other non-DOE contractors.

Mr. **Fuqua**. You have about a $6.58 million increase of a $21 million program, about a 45-percent increase. How much is that to fund new proposals in the long-range research program for large-scale scientific computers?

Dr. **Trivelpiece**. It is approximately $7 million, which would be the new funding for a parallel processor and software development and some small hardware activities.

Mr. **Fuqua**. There has been some concern expressed in the media—you can take that any way you wish—about the university research reactors using highly enriched uranium and causing an undue safety and security risk. As a matter of fact, there was an article in the Los Angeles Times back in late January. Is that a concern, or does it have any validity?

Dr. **Trivelpiece**. I think the matter is in the hands of the Nuclear Regulatory Commission. It is true that we do have university research reactors, and we are responsible for quite a few of them, and we do provide the refueling for them, and quite a few of them do use highly enriched fuel.

Mr. **Fuqua**. And quite a bit of the funding.

Dr. **Trivelpiece**. Some of the original funding, although many of them are operated by the institution and we simply provide the refueling now. But in any event, there are some of them that do have highly enriched uranium in them, and the Nuclear Regulatory Commission is reviewing that at the moment. There is a strong possibility that they will issue a ruling which would require us to convert those to low-enriched fuels. Should that occur, we would have to review those that can do it and what the cost would be and what the impact on the institutions would be.

Some of the reactors are permanently fueled, in effect. From my point of view, it would not seem to be appropriate to take out the fuel of those that have been permanently fueled. But there are some for which it would be relatively straightforward to convert them from highly enriched fuel to lower enriched fuel.

Mr. FUQUA. In the budget request for basic energy sciences, the budget request of $419 million reflects about $3 million for savings resulting from management initiatives in the area of administrative processes and field structure. What specific initiatives have resulted in these savings?

Dr. TRIVELPIECE. As you know, this is part of the President's Private Sector Survey on Cost Control, and the Department of Energy was requested to effect savings of some $96 million across the activities. By the time that requested saving was distributed down to the various program elements, BES' portion of this is $3 million. I think in the spirit with which this is done, it is our intention to have the laboratories and have the university programs do the work they are doing. There will be no change in scope, but by efficiencies which they are expected to effect at their own organizations, they are to be able to do what they are doing on $3 million less spread across the $419 million. It is not a large reduction, and it is part of the President's program.

Mr. FUQUA. Thank you.

Mr. Gregg.

Mr. GREGG. Thank you, Mr. Chairman. Following up on the supercomputer issue, do you interface at all with NSF's supercomputer initiatives which they are picking up?

Dr. TRIVELPIECE. We are in communication with them. There was a committee that was started through the Office of Science and Technology Policy, the Federal Coordinating Council on Science Engineering and Technology, to look into the access problem and the next generation of supercomputers, as well as the fifth generation technology issue. As a result of that, there is a committee which is still in existence and it has made some reports, and those reports have been incorporated in the testimony given here earlier at another hearing. We do coordinate with them. We are aware of what they are doing. As I have said in my own testimony previously, the access problem in the United States for scientists at our laboratories and universities to class 6 systems is so pervasive and so large that we should do something, NSF should do something, and NASA should do something. I do not think we are at any risk at the level of request which the President's budget incorporates across the various agencies of overkilling this problem, at least not this year.

The $20 million that is requested by the National Science Foundation I certainly believe is appropriate. They are capable of supporting activities that we are not, because we are enjoined to support only our own contractors. Our contractors do include a large segment of the university community, and we certainly will take advantage of this opportunity to do that. But we do not coordinate them in the sense that we put all our proposals on the table and interleave them or exchange them in any practical sense. But we do coordinate with them.

Mr. GREGG. You said it was going to be a Cray computer?

Dr. TRIVELPIECE. There is a certain necessity to be circumspect, in view of the competitive procurement situation in the United States. Certainly, the class 6 computers in the United States include the Cyber 205 and the Cray 1 and its subsequent versions. Whether other computer vendors will come along that will supply apparatus that is equal to or better than that, and whether or not we would purchase it, I think remains to be seen at the time that the procurements are made.

Mr. GREGG. Could there be a Japanese computer that you might buy?

Dr. TRIVELPIECE. I think that would again depend on the circumstances. Certainly the Japanese are supplying computers whose current operating speeds are approaching those or equal to those of the Cray and the Cyber. Whether or not the Buy America Act and other constraints would influence the decision to buy Japanese computers or not, I do not know. It would depend on procurement issues, but they are certainly in a position to supply equipment that would be difficult to ignore from its performance capabilities.

Mr. GREGG. Shifting focus, you are doing some research on acid rain?

Dr. TRIVELPIECE. Yes; we do research, not the basic energy sciences program. That is carried on under the biology and environmental research program, which would be the subject of another hearing. Congressman Scheuer is the chairman of the subcommittee to whom we normally would testify with respect to the acid raid programs. But I am reasonably familiar with it and would be happy to answer any questions you might have.

Mr. GREGG. I was just wondering if you could tell us what your plans are.

Dr. TRIVELPIECE. DOE's activities in the acid rain programs have to do with more of the basic research, trying to characterize what comes out of the various stacks, what is its chemical composition, what does it do when it gets into the atmosphere, how is it transported from one place to another. Once it reaches the biosystem, what does it do, and what is its influence on the ecosystems.

The experiment which is being requested this year which is called CAPTEX, cross-Appalachian tracer experiments, and the nonlinear experiments which we are doing or proposing, $5 million is being requested for that, and that is a question of whether or not there is a direct linear proportion between what goes down and what goes up. There are some subtle chemistry issues associated with that.

By and large, we are not involved directly in energy research. We are part of the Department, and any of the policy issues surrounding the acid rain concerns—you know there is something called an Interagency Task Force on Acid Precipitation, in which the Department of Agriculture and NOAA and the Environmental Protection Agency have the lead. DOE is one of the members of that task force, and as such we are involved in some of the assessment issues of what goes on with acid rain. We also are doing some of the research.

Elsewhere in the Department, there is the abatement and control issue, which is being addressed through fossil energy, and I think there is something on the order of $26 million in new money that fossil energy has that is devoted to the control and abatement strategies with respect to fossil plants and trying to reduce the amount of effluent containing sulphur emitted by them. But that is not a program for which I have any responsibility.

Mr. GREGG. What is your timeframe for the cross-Appalachian study?

Dr. TRIVELPIECE. That has been started. I am not sure what the conclusion of that is. I did not review that specifically in connection with this morning's hearing. I think it is a 2- or 3-year program, but it has been started. It involves some hydrocarbons that can be traced accurately, and they are released from a number of points in the Ohio Valley and vicinity, and then they are picked up elsewhere.

There are several problems. One is just the so-called connection matrix. Namely, it comes from here and it goes to there. What is the connection between this point in geography and that point in geography. Then, once you have established that, there is a question of what does nature do as the chemical constituents are modified by the atmosphere, by sunlight, by other pollutants that are in the area, and that is the transition chemistry problem. Then once it gets to the other side, what does it do, and there are specific issues about the ecology of various lakes, what it does to the forest canopy, what it does to the ecosystem in general.

We are involved in various aspects of that, but I think the timescale for the cross-Appalachian tracer experiments is about 3 years.

Mr. GREGG. Thank you.

Mr. LEWIS. I have no questions at this time.

The gentlelady from Rhode Island, Mrs. Schneider.

Mrs. SCHNEIDER. Dr. Trivelpiece, I was looking through some material here. Under the chemical sciences subprogram, the administration proposed the funding request for capital, equipment, and construction, basically general purpose equipment, $2 million for Argonne National Laboratory; and in general purpose projects, there are a whole series of them for Argonne and Ames and Notre Dame, and so on. This construction project data sheet states, and I would like to quote from here so I am sure to get it right:

> Included in our request for the first time in 1985 is full general purpose project funding for the Argonne National Laboratory. Previously landlord responsibility at this laboratory has been with the nuclear energy breeder program, but program shifts and restructuring necessitates the shift of this responsibility to the BES program.

I was wondering how that decision was made and who recommended this shift to take place.

Dr. TRIVELPIECE. This was discussed a little bit earlier here in the hearing.

Mrs. SCHNEIDER. I regret that I was late.

Dr. TRIVELPIECE. The Department has tried to look at the issue of general plant equipment and general plant projects across the board and not to have them addressed on a piecemeal basis. To do this, we are doing it through what is called the Laboratory Management Council. The decision to coordinate this through basic energy sciences rather than through the nuclear program was reflected by the fact that the nuclear program had reduced this amount to about $250,000 previously.

There were two things that were done. One was to try to raise the GPP level back up to levels consistent with the overall investment in Argonne Laboratory. The other was because of the size of the BES program at Argonne, to use it as the landlord responsibility. The Department uses one program at each laboratory to put the entire budget for the GPP/GPE category in it, rather than having it allocated across many programs, in which case then you would have no opportunity unless you put together a very complicated crosswalk table, to discover just how much we were putting into this category at a given laboratory. So it is a matter of management practice to put it in one institution. The decision to do this was made with the Laboratory Management Council in the Department.

Mrs. **Schneider**. The normal general purpose project requirements at Argonne National Laboratory seem to have deteriorated to such a point that a major budget increase is required for 1985 to meet minimal laboratory requirements. How and why did that occur? If this was to be maintenance money, how is it that essentially you were able to eat your seed corn?

Dr. **Trivelpiece**. It is not quite the same as routine maintenance. These are at a slightly higher level than what I refer to as ordinary maintenance. These are projects that are required to maintain the laboratory. As I said earlier this morning, there is almost a natural and unfortunate conflict-of-interest that is imposed on program managers at every level in institutions such as the department.

That is, in a given year, if there are budget stringencies, should you take action that results in people being terminated from the programs, or should you let the roads go 1 more year. I think unfortunately the tendency always is to let the roads go for 1 more year. You can do this for a few years, but eventually the roads get pretty bad.

So the plan here is to try to recognize that this has been a problem, elevate it to a corporate level within the Department, and try to make a uniform approach to the GPP, GPE category at all our laboratories to reflect the investment that has been made in them and to keep them operating at an appropriate level and maintained properly.

Mrs. **Schneider**. Very fine. Thank you, Mr. Chairman.

Mr. **Lewis**. The gentleman from Iowa, Mr. Harkin.

Mr. **Harkin**. Thank you. I have a couple of questions of Dr. Trivelpiece.

How much of the BES program's funding is going to support facilities such as the National Synchotron Light Source and the Combustion Research Facility?

Dr. **Trivelpiece**. I do not remember the exact numbers. Perhaps Dr. Kropschot would like to answer that.

No. I am surprised I do not know it, and I am surprised they do not know it. The National Synchotron Light Source total is about $20 million.

Mr. **Harkin**. What about the Combustion Research Facility?

Dr. **Trivelpiece**. $6 million for the Combustion Research Center.

Mr. **Harkin**. Is the increasing support for facilities squeezing out the numbers of individual researchers supported by BES?

Dr. **Trivelpiece**. No.

Mr. **Harkin**. Are we supporting fewer researchers at all? Are we having a problem with fewer researchers at all?

Dr. **Trivelpiece**. Not that I am aware of. It has been more or less constant. The attempt has been to try to operate the facilities and make them available to individuals. We do not pay for the support of all the individuals that take advantage of the facilities. For example, the National Synchotron Light Source is used 20 percent by DOE laboratory personnel at Brookhaven and 40 percent by universities and 40 percent by industry. Industry uses the facilities, but they pay their own way there. Not only that, they also supply rather expensive equipment, which is part of the agreement that they make available to other researchers than themselves and eventually they walk away from and leave as a legacy to the laboratory to be used by other universities. In some cases, the universities' researchers there are being supported by the National Science Foundation and other agencies.

Mr. **Harkin**. You made mention to one of Mrs. Schneider's questions about the roads being a secondary consideration. How much equipment do you have mothballed or set aside of an expensive nature that is not being used? What percentage?

Dr. **Trivelpiece**. I have no way of answering that question from memory. I do not know the answer, but I would be glad to try to determine what the answer is. I hope it is not very much. In any event, there is a systematic process by which apparatus that the laboratories have that is no longer of direct need to the laboratories is made available on a surplus basis. Quite frequently, as I have gone around and visited university laboratories, people have pointed out to me that this is the old Astron tank here, and this is somebody else's vacuum pump from one of the laboratories. It is made available, and I think it probably has a life far beyond that which was ever anticipated by the original designer, as well as utilization for quite a few rather interesting scientific purposes. Old equipment does not die; it just gets relocated.

Mr. **Harkin**. I have one final question. Do you feel that the Office of Energy Research is moving in as strong a position as it can for research into alternative energy sources?

Dr. **Trivelpiece**. It is a qualified yes. We are the basic research end of the Department's activities. So, if you try to ask what is the direct cause-and-effect relationship between a watt, a kilowatt saved next year in an activity which takes places this year, I would be hard pressed to make an appropriate comparison. On the other hand, if you take a longer time base to look at these things, I think yes, the kind of research and biological energy research, in which you are trying to understand how photosynthesis works, can we make a nonbiological photosynthesis activity take place and what would happen there. In fact, you will hear from Dr. Pimentel; he is one of the experts in this. You might like to ask him about that particular scientific area.

But I think there is a connection between the activities we do and what will be improvements tomorrow in terms of the reduction of friction, the kinds of ceramic things that were mentioned earlier, the new materials, the nickel aluminide I mentioned in my opening remarks, the high temperature material which will permit operation of facilities in a more efficient manner, with longer-lived material, utilizing cheaper initial ingredients that will come into being.

So on the whole, I think the answer is yes. The specific cause-and-effect relationship in a given year-to-year basis is very difficult to establish.

Mr. **Lewis**. Mrs. Schneider, you had a question from yesterday you wanted to ask?

Mrs. **Schneider**. Thank you. Actually I have two questions. One was, I was hoping that you might be able to update us, as you had mentioned yesterday, on the nuclear waste basic research that you are involved in.

Dr. **Trivelpiece**. That activity is somewhere in the neighborhood of $5 million in the basic energy research program. It involves this general concern. If you have waste material of a nuclear nature, it has its own spontaneous radioactivity. That radioactivity influences the chemical character of that. Does that influence its migration and so on through rock and rock formations. We are concerned with things like neptunium in basalt, and the fact that it does not migrate as fast as it might otherwise as a result of some attachment that takes place chemically.

We are engaged in various basic research activities that look at what happens to containers, what happens to the waste, where does it go, how does it migrate, how can you keep track of it and the like. It is not a large part of the Department's activity, but it is on the basic end of the spectrum.

Mrs. **Schneider**. But we have been studying the basic makeup of various geologic options for a number of years now. I am just wondering, I have not heard any conclusive research being presented anywhere. I do not know that we are any further ahead today than we were 10 years ago in basic research, in determining how quickly the various forms of nuclear waste might be moving through basalt or whatever.

Dr. **Trivelpiece**. From a technical point of view, my opinion is that there is a satisfactory solution to the waste problem. It, of course, is a very contentious political and social issue as to how to handle the nuclear waste, both that which has been generated from weapons programs as well as that which will be generated in civilian nuclear power programs. But airplanes are a good example. Boeing has not stopped doing basic research on aerodynamics because it happens to build very superior aircraft for transport, both military and civilian. The research that we are doing is the sort that I think should continue, even if we already had a waste repository going and waste stored in it and everyone was in a politically and socially happy mood with regard to the Nation's nuclear waste. This is the kind of activity that should go on almost indefinitely at some level.

Mrs. **Schneider**. I understand the feeling of your support for continued research, but I think that considering the quantity of waste that we are continuing to generate, the solution that we have now seems to be more of a stopgap measure. I guess we are looking to move beyond that interim space, to a point where we can feel that we have found ourselves in a situation where we can appropriately dispose of it.

Dr. **Trivelpiece.** Our citizens need to be satisfied that the approach we have to handling nuclear waste is acceptable.

Mrs. **Schneider.** I guess that is the problem. There are a lot of citizens who are not content that we are handling it satisfactorily.

Dr. **Trivelpiece.** That is true, and that certainly is one of the problems. But we do have nuclear waste now. It can be handled in, I believe, a safe manner. It does get into the debate on whether or not it can remain immobilized for periods of thousands or tens of thousands of years. The debate tends to focus on that. Certainly, we do understand a great deal about how to contain it, what it does in the containers; if it does get into the ground system, how it migrates, and so on. But we can afford to know a great deal more about it. In the meantime, I think there are practical solutions that should, in my opinion, be acceptable to the public but they clearly are not.

Mrs. **Schneider.** I can understand the scientist's perspective, for a number of obvious reasons, but I think that my colleague will agree that we, as Members of Congress, very much have to be task-oriented. We like to produce. Based on his earlier question, which was to what degree are we involved in basic research for alternative energy supply, here, again, it seems very frustrating that we cannot seem to go back to our constituents and say, "Look, we have A, B, C, D, and E. These are major discoveries that we have made to improve energy efficiency or to supply you with greater energy."

I think that oftentimes we have a great deal of frustration that we are funding research, for example, although now the budget is really minimal, but we do not seem to be getting too far. Or if we are, we have a real problem with technology transfer of information. I think that if I were to walk down the street in my district and ask my constituents to name some of the latest inventions or developments insofar as energy efficiency is concerned, maybe they would say the showerhead that would use far less of your hot water than might something else. But other than that—If we are making advances, which is my first question—Are we?—then where is it, and where is the practical application for the consumer?

Dr. **Trivelpiece.** I think there are incremental advances. Breakthrough or discovery is probably not the appropriate term to apply to this particular type of activity. Certainly improved efficiencies in small terms make a great deal of difference. The physics and chemistry of flame and combustion—although flame is one of our older tools that mankind uses, we still have a rather imperfect knowledge as to what goes on in terms of the simple combustion involving natural gas and a mixture of air and how turbulence affects that. The Combustion Research Center's activities have made rather impressive progress in understanding the efficiency of combustion and the byproducts and so on. The lime injection multistage burner activities are reducing the amount of effluent that is produced in the stack gas that comes out from coal plants. Part of that is attributable to activities that took place in the Combustion Research Center.

There are a number of these, but they are not in any sense of the word dramatic. They are all small incremental improvements, and I think that is just the result of the character of the activity. The kinds of things that get attention, get Nobel prizes, you know about them; I do not have to come up here and testify about them. I would be happy to try to task the people who work with me in the Department to provide some summary of these in a way that might satisfy your concern, but I believe it will be a large collection of small things rather than a few dramatic items.

[The material referred to follows:]

Some Examples of Accomplishments Under the Basic Energy Sciences Program during 1983

(February 15, 1984)

The Basic Energy Sciences Program supports about 1200 research projects. The following selections, while not fully reflective of the full range of activities under the program, are examples of how basic research can contribute to solving a wide variety of energy problems.

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1. Control of Structure and Properties of Ceramic Surfaces by Ion Implantation Shown

It has been demonstrated that the structure and surface hardness of ceramic surfaces can be modified and controlled by means of ion implantation to yield surface hardnesses that are greater or less than that of the original ceramic.

Results for ion-implanted alumina showed a hardness increase of 15 to 50% and a scratch-wear resistance increase of 30% as a consequence of ion implantation with chromium, nickel, iron, titanium or zirconium ions. The principal mechanism of implantation hardening was found to be due to implantation-induced structural damage on the aluminum sublattice, with some contribution from implantation damage on the oxygen sublattice.

The hardness also can be made to decrease during post-implantation thermal annealing of aluminum oxide; the mechanism was found to be associated with the recovery of the implantation-induced damage on both the aluminum and the oxygen sublattices. The implantation of alpha-phase silicon carbide with chromium or nitrogen caused the implanted surface region to become amorphous at implantation fluences above a certain critical level. This transformation from the crystalline to an amorphous state is accompanied by a decrease in hardness of 15 to 25%, an increase in fracture toughness of 30 to 40%, and an incease in scratch wear resistance of up to 70%.

This work established the feasibility of using ion implantation to systematically alter the structure and properties of ceramic surfaces. It has also demonstrated that control of the resultant structure may be achieved by the variation of implanted ion species, implantation temperature, and post implantation heat treatment.

(Oak Ridge National Laboratory, C. J. McHargue, B. R. Appleton, C. W. White, and J. M. Williams)

2. Selective Catalytic Conversion of Methanol to Ethanol Discovered

A new catalyst system has been discovered for conversion of methanol to ethanol. The system has several practical advantages over existing methods. Starting with methanol produced from coal, dry ethanol, which has higher fuel value per unit volume than methanol, is produced. The catalyst is based on iron pentacarbonyl in the presence of a tertiary amine. The principal co-product formed is carbon dioxide, rather than water as in existing methods which use a cobalt/carbonyl catalyst. Eliminating water is particularly beneficial because it can save the costly drying step.

In addition to not producing water, the iron system catalyzed reaction only requires half as much expensive hydrogen as in the cobalt/carbonyl catalyzed system. The selectivity of the iron/amine catalyst is virtually 100% for converting methanol to ethanol. There are no higher alcohols, alkyl acetates or acetals formed, in contrast to the cobalt systems, and this simplifies product purification considerably.

A mechanism for the iron/amine catalyzed reaction has been established through detailed chemical and kinetic studies. This understanding has led to development of a mixed catalyst, $Mn_2(Co)_{10}/Fe(Co)_5$/amine, which has both activity and selectivity superior to either metal carbonyl alone.

(Argonne National Laboratory, J. W. Ratkhe & coworkers)

3. Glow Discharge Implanted, Laser Annealed Silicon Single Crystals Produce Simple, High Efficiency Solar Cells

Simple, low-cost, yet very high efficiency solar cells have been produced from single crystal silicon by glow discharge implantation doping followed by pulsed laser annealing. This method involves two well understood processing steps, is easily automated and could radically change the manufacture of solar cells.

The cells are fabricated from standard phosphorous-doped single-crystal silicon wafers. A p-n junction is formed by implantation of boron followed by pulsed high-power laser illumination to activate the implanted atoms and anneal any implantation damage. A back surface field is created to reflect minority carriers back to the p-n junction area by deposition of a thin layer of antimony followed by illumination by laser pulses to cause inward diffusion. The cells are completed by cutting the wafers into desired sizes, applying contacts and antireflection coatings. The process is simple, though subtle, and efficient. It uses laser annealing and an inexpensive glow discharge boron implantation technique, both of which are easily automated and capable of high production rates. There is no high temperature processing, which is usually difficult and poorly controlled.

This development has led to three patent applications, two of which already have been granted, and the development of a XeCl laser system by an American company for automated high-production rate laser processing of these solar cells. Efficiencies of about 16.5% for these cells were measured by the Solar Energy Research Institute and found to be higher than that of any solar cell ever tested under the same conditions.

(Oak Ridge National Laboratory, R. T. Young & coworkers)

4. New Thin Film Photoelectrode Uses Visible Light to Generate Electricity or Split Water

One micron films of intrinsic (undoped) amorphous hydrogenated silicon deposited on stainless steel have been investigated as photocathodes in photoelectrochemical cells. The hydrogenated silicon was synthesized at RCA and its behavior characterized at MIT. The photoelectrodes are rugged, efficient and inexpensive.

The efficiency of the photocathode for converting visible light to electricity is in the 1-2% range, which is only about one-third less than efficiencies attained using expensive single crystal electrodes under the same conditions. Even more promising is the observation that this type of electrode produced a photovoltage more than 50% greater than that produced using a single crystal electrode. The efficiency for generating hydrogen by photoassisted electrolysis of water is equal to that obtained with the best single crystal electrodes.

Many advances reported in photoelectrochemical energy conversion in the past two years have been obtained with use of ultraviolet light, a less intense part of the solar spectrum at the earth's surface. This set of advances, in contrast, used the much more abundant visible part of sunlight. Research continues to increase further both our scientific understanding of these phenomena and the efficiencies of functioning of the new type of electrodes.

(Massachusetts Institute of Technology, M. Wrighton)

5. First Mu Meson Catalyzed Fusion Reaction Rate Measurement

In conventional approaches to fusion, hydrogen gases are heated to extremely high temperatures to form a plasma so that fusion reactions occur, releasing energy. Thirty-five years ago, it was suggested (by F.C. Frank and independently by Andrei Sakharov) that an elementary particle known as the muon could serve to catalyze the hydrogen fusion reaction so that it could proceed without the need for high temperatures. This process is therefore called cold fusion or muon-catalyzed fusion.

The basis for muon-catalyzed fusion is as follows. The negatively-charged muon behaves like a heavy electron and can substitute for an electron in a hydrogen atom. The muon is 200 times as heavy as an electron, and because there is an inverse relation between the mass of the negative particle and the radius of the atom, the muonic atom molecule is 200 times smaller than an ordinary hydrogen atom. The reduced size of the muonic atom brings the hydrogen nuclei so close together that they interact and fuse very soon after the muonic molecule forms. Indeed, the conditions inside a muonic hydrogen molecule are similar to those found inside a white dwarf star!

In this research, muons are introduced into a mixture of hydrogen gases (deuterium and tritium). Gas temperatures range from -280° F to 530° F, so the gases are very cold compared to plasmas. The muons replace electrons to form muonic hydrogen molecules and fusion ensues immediately. The muon is then free to catalyze other fusion reactions. Up to seventy (70) fusions per muon (average) have been observed in initial experiments. This is greater than expected but still insufficient for net power production. It has also been observed that the rate of the reactions increases with temperature (up to 530° F so far). However, it is clear that no thermal runaway or explosion is possible with this process.

Muon-catalyzed fusion research is continuing with Department of Energy support and similar research is also beginning in Europe and the Soviet Union. The research will provide answers to recurring questions regarding the possibility of practical applications for muon-catalyzed fusion.

(Idaho National Engineering Laboratory, S. Jones)

6. Soot Formation at Elevated Pressures Studied Using Laser Probe

Using advanced laser diagnostic techniques, considerable advances are being made in understanding the complex phenomena involved in the behavior of flames. The formation of soot, the familiar particulate matter resulting from incomplete combustion, is not only a serious source of reduced efficiency during combustion, but a potential environmental hazard as well.

Although there have been extensive studies of soot formation in combustion systems, most investigations have been carried out at normal or atmospheric pressure, despite the fact that, in practice, soot formation is most often a problem in systems that operate at high pressure. Applying advanced laser techniques, direct evidence has been obtained that soot formation increases at high pressures, not because the particles become larger, but because there are more of them.

While flames at elevated pressure are similar to those at normal atmospheric pressure, they become more compact as pressure increases. It was found that, with increasing compactness of the flame under pressure, the number of soot particles formed increases considerably. The experimental evidence comes from the much greater reduction in intensity -- by a factor of about 400 -- of a laser beam as it passes through a soot laden flame at two and one-half atmospheres of pressure compared to a soot laden flame at normal atmospheric pressure. Particle size very much affects the scattering of the laser light, and the ability to distinguish between either larger particles or more particles being responsible for the reduced beam intensity is dependent on sophisticated scattering measurements and their interpretation.

This study is typical of those now permitted by the advanced techniques for combustion research available at the Combustion Research Facility and has produced some important insight into the fundamental mechanisms responsible for the increase in soot production with pressure. Results such as these will ultimately provide the understanding necessary to control soot production in practical combustion devices operating at elevated pressure.

(Sandia National Laboratories-Livermore, W. Flower, and Stanford University, T. Bowman)

7. Highly Accurate Method for Isotope Ratio Measurements Devised Using Selective Ionization

A new, highly-selective method for measuring isotope ratios has been developed. The method, termed resonance ionization mass spectrometry (RIMS), is uniquely suited to the measurement of isotope ratios in situations where interferences from other elements are present. These interferences arise in mass spectrometry because ions are separated and detected according to mass. The problem of different atoms with the same mass occurs in both the lanthanide rare earths (e.g., cerium, used in color TV tubes, and neodymium) and actinide elements (e.g., uranium and plutonium). Resonance ionization is very selective, producing ions of only one element at a time, thus removing interferences without resorting to chemical separations or artificial measurement conditions, which seriously impair precision.

Research thus far has focused on the system cerium:neodymium:samarium (Ce:Nd:Sm) because Nd is an important element in nuclear reactor fuel burn-up analysis. Interferences from Ce (mass 142) and Sm (masses 144, 148 and 150) must be eliminated in order to arrive at an accurate isotopic analysis of Nd.

A high-powered nitrogen laser and a dye laser are used to produce light pulses of the proper wavelength to ionize Nd selectively in the presence of Sm and Ce. The ions thus formed are mass analyzed in a mass spectrometer. By switching the spectrometer back and forth between two masses, an isotopic ratio can be measured. The results obtained for isotopic ratios of Nd and Sm can be compared to the results from ordinary mass spectrometry taken under the same conditions. Errors of several hundred percent have been reduced to 1-2% with the new measurements!

(Oak Ridge National Laboratory, Dr. D. Donohue, Dr. J. Young)

8. Shear Added as a Variable to Equation of State for Fluids at Very High Flow

It has been found by techniques of molecular dynamics that in fluids, under conditions of very high flow, the equation of state includes a term involving shear as a parameter along with the usual variables of temperature, pressure and volume, necessary to define the intrinsic properties of a fluid.

Equations of state are used to predict the properties of fluids, including thermodynamic properties which are, in turn, used in the prediction of fluid behavior and the design of chemical processes. The discovery of the shear effect offers an explanation of previously unaccounted for observations of phase changes occurring under conditions of high shear. This discovery is expected to make it possible to predict thermophysical properties of complex fluids under conditions of unusual shear. Heretofore, there has been no awareness of the "shear" term because it makes essentially no contribution in the equation of state under normal conditions. Under conditions of very high flow or extreme mixing of a fluid, shear is high enough to have an effect.

The consequence of the shear effect is illustrated by the nitrogen-ethane system in which a region of non-miscibility, or a miscibility gap, is predicted by "normal" theory at given conditions of temperature and pressure, but disappears entirely when shear is taken into account. The nonexistence of a miscibility gap has significant practical consequences.

(National Bureau of Standards, H. J. M. Hanley - jointly supported by NBS)

9. The Effects of Mt. St. Helens and El Chichon Volcanos on the Stratosphere are Significantly Different

It is known that volcanic eruptions can change climate by injecting gas and dust into the stratosphere. Of the two components, volcanic dust usually has the shorter residence time in the stratosphere (up to several weeks) while the gas, consisting mainly of SO_2, is more gradually oxidized to sulfuric acid (H_2SO_4) and other sulfates that nucleate and grow to stratospheric aerosol particles capable of affecting the solar radiation balance of the earth.

The effects of the El Chichon, Mexico eruption of 1982 and the Mt. St. Helens activity of 1980 have been sorted out from solar radiation measurements taken with a computer-controlled radiometer developed at the Pacific Northwest Laboratory.

Although Mt. St. Helens produced a large spike of SO_2, its conversion to sulfate particles was rapid and the stratospheric aerosol injection was short-lived. Consequently, no long-term effect on weather is expected from stratospheric loading by St. Helens.

The pattern of aerosol development associated with the El Chichon eruption of April 1982 was quite different. Over middle northern latitudes, where the measurements were made, the first influx of stratospheric aerosol particles did not appear until September 1982, where an abundance of sub-micron sized particles was measured. The size of the particles has since grown steadily to approach a relatively large average diameter of one micron. The larger than expected size of the sulfuric acid particles and their long residence time may well change insolation and thus have climatological consequences.

(Pacific Northwest Laboratory, J. Michalsky)

10. Wear in Sliding Friction Shown to be Due to Surface Oxidation

A wide variety of systems have components such as clutches, brakes and commutator brushes where one surface slides over another with little or no lubrication. In such systems, different types of friction induced vibrations have been frequently observed. The squeal and chatter they produce can cause excessive wear of components, severe surface damage, and fatigue failure in addition to objectionable noise levels. Research on the underlying damage mechanisms has been focussed, in particular, on interactions between friction-induced vibration and wear.

Recent experiments have shown more clearly than ever before that mild wear is due to surface oxidation. Mild wear in this context refers to wear over the range of speeds and loads normal for use of sliding contacts between metals in dry (i.e., unlubricated) conditions. The experiments showed that formation of wear particles in mild wear is localized in the oxide film formed on the surface and is due to a fatigue mechanism. Further, mild wear was shown to be a function of the system rigidity that determines the frequency of slider oscillation and, hence, the number of loading cycles. The experiments also defined the conditions leading to the transition from mild wear to severe wear.

(Illinois Institute of Technology, S. Kalpakjian)

11. Tumor Forming Gene Eliminated in Widely Used DNA Vector in Plants

One of the impediments to "genetic engineering" in higher plants has been the lack of a suitable vector (a vector is an agent that can "carry" the desired gene) for transferring desirable genes into target plants. The candidate vector most studied has been a plasmid (DNA segment) deriving from the bacterium Agrobacterium tumefaciens. The plasmid (Ti) may be used to transfer pieces of DNA carrying specific genes into host plants. Several problems exist in using this vector, however one of these is having the genetic message carried by the Ti plasmid into the host expressed in the host, i.e., having the genetic message translated into a protein in the host possessing the ability to catalyze specific chemical reactions. Another is that the plasmid itself when introduced into the host plant causes tumors to develop in the plant.

Within the past year work has progressed to the point where it is now feasible by genetically altering the Ti plasmid and its introduced genetic message to eliminate tumor formation (called "disarming" the plasmid). Furthermore it is also possible to demonstrate the expression of an introduced genetic character in host plant cells. Three laboratories, two in the U.S. and one in Europe, conducted these experiments, to "disarm" the Ti plasmid and to demonstrate the new genetic character, independently and obtained similar results. This information brings the day closer to when it should be possible to introduce desirable traits into recipient plants with the objective of improving cultivated species.

(Washington University, M. D. Chilton)

12. Uranium Proven Unreliable Substitute for Transuranic Elements in Simulated Nuclear Waste Glass Studies

A study of simulated radioactive waste glass forms using uranium to substitute for transuranic elements has shown that they do not provide a reliable simulation of the structure and bonding properties of transuranics in silicate glasses. Since the leaching properties are dependent on bonding, this result indicates real waste systems must be investigated for reliable prediction.

To investigate the leaching behavior of radioactive waste forms, it is a common practice to study nonradioactive uranium analogs in order to simplify experimental procedures. For glass forms, air melted uranium glasses are generally studied which contain U^{6+} ions only. The assumption is made that the transuranic glasses will behave much like the uranium analogs. However, this procedure appears to be highly suspect, since transuranic glasses exhibit properties that are more similar to U^{4+} than U^{6+} glasses, and the results of EXAFS and X-ray photoemission experiments, and complementary investigations of the solubility and other phyhsical and chemical properties, have shown very different bonding characteristics of U^{4+} and U^{6+} ions in glasses. The important practical consequence of this research is that it demonstrates the unreliability of the usual simulation investigations of leaching in aqueous environments, where air melted glasses containing U^{6+} ions are used to simulate the same glasses containing transuranic elements

(Argonne National Laboratory, D. Lam)

13. Scientific Method Established for Assessing Hydrogen Donor Capacity of Solvents for Coal Liquefaction

A new procedure has been developed to assess how effective various solvents might be as sources of hydrogen in coal liquefaction. Liquefaction of coal involves breaking chemical bonds between carbon atoms and increasing the hydrogen content to establish more liquid-like properties in the system.

Since well established chemical principles involving bond dissociation energies form the basis of the new procedure, it can be used reliably to guide the production of better hydrogen donor solvents.

In this new procedure, a reactive chemical fragment, the orthoallylbenzyl radical, is generated by thermally decomposing the chemical substance orthoallylazotoluene. In the presence of a hydrogen donor or coal liquefaction solvent, this radical can either abstract hydrogen from the donor solvent or undergo an intramolecular rearrangement reaction. The two processes form two very different hydrocarbon products. Measurement of the yield or concentration ratio of these two products allows direct comparisons to be made of the hydrogendonor capacity of potential coal liquefaction solvents: the greater the yield of the chemical resulting from hydrogen abstraction, the better the donor capacity of the solvent.

The hydrogen donors studied thus far show expected trends of greatly increased rates of abstraction as the bond dissociation energy of the donor compound drops. The method is currently being applied to a wide variety of donor molecules and is ideal for the characterization of hydrogen donor solvent quality.

(Pacific Northwest Laboratory, J. A. Franz & Coworkers)

14. New Superconducting Shielding Method Reduces Magnetic Fields to Extremely Low Level

A new superconducting magnetic shielding method capable of reducing ambient magnetic fields to the nanogauss level has been demonstrated. This technique has the potential to revolutionize the methods of obtaining low and stable magnetic field environments necessary for low-noise operation of sensitive superconducting devices such as the Josephson Junction computer.

The method can be used to suppress magnetic fields to less than 10^{-10} Tesla, about one-half of one-millionth of the average magnetic field on the surface of the earth. This method can suppress magnetic fields more reliably and to lower values than any known technique. A very important utilization would be the shielding of such devices as computers which use superconducting elements from magnetic fields. During the necessary cooling down to operating temperatures near 4.2° Kelvin, any magnetic field may cause the sensitive superconducting circuit elements to malfunction.

This technique uses superconducting materials and some of their less obvious properties to remove and shield a region of space from magnetic fields. Superconductors exhibit the Meissner Effect: as a material is cooled below its superconducting temperature, it will expel the magnetic field. However, if the material is not a simple pure superconductor - and most practical materials are not - there will be "pinning sites" where some magnetic flux is trapped. Nearly twenty years ago, magnetic fields were shown to be quantized in units of about $2x10^{-11}$ Tesla. Thus each pinning site will trap an integral number of flux units. However, if a sufficient electrical current is passed through the superconductor, more than the "critical depinning current," the flux quanta become depinned and can be swept to the edge of the superconducting material.

This new superconducting magnetic shielding technique utilizes these fundamental properties to sweep the magnetic flux quanta from a long cylinder of a superconducting metal and thereby produce and maintain a region of space at the center of the cylinder at low or no magnetic field.

(Ames Laboratory, J. Clem)

15. First Measurement Made of Metallic Vapor Pressure of Einsteinium

The first measurement of the metallic vapor pressure of the man-made element number 99, einsteinium, has been made using material produced and prepared in the High Flux Isotope Reactor and Transuranium Processing Plant at the Oak Ridge National Laboratory. This is the heaviest and also highest atomic number element for which this fundamental thermodynamic measurement has been made. From the experimental data the investigators have derived a value of 31.2 kilocalories per gram-molecular weight for the energy required to vaporize the metal from a solid to a gas. This information is valuable for the increase in our understanding of the fundamental chemical and physical properties of elements and of their behavior in chemical reactions.

The measurements indicate that Einsteinium is a divalent metal, like calcium and magnesium, and thus quite unlike the lighter actinide element metals. This confirms earlier predictions based on the observed trend in the higher actinides, of the increasing stability of the divalent as compared to the trivalent state.

Einsteinium may well be the last element in the Periodic Table for which this type of measurement can be made because the next higher element, fermium, can thus far only be produced in hundred-million-fold smaller quantities.

(Los Alamos National Laboratory, J. Ward, and Oak Ridge National Laboratory R. Haire)

16. New Downhole Probe Measures Fluid and Heat Flow Simultaneously

As drilling for scientific purposes and for energy and material exploitation penetrates into rocks of increasingly hostile and variable properties, it is necessary to develop downhole measuring tools with enhanced capabilities. The measurement of heat flow in holes drilled through permeable rocks containing fluids can be a problem because it is difficult to sort out convective effects due to fluid flow from the effect of heat conduction through the rock itself. A research team focusing on new in situ downhole geophysical measuring techniques has developed an instrument capable of measuring and distinguishing between these two heat flow mechanisms.

The method depends on using a controlled heat source lowered into the hole to disturb the ambient heat flow regime in a reproducible way. In addition to a heat source, the instrument also has an array of temperature measuring devices (thermistors) that monitor the response of the natural environment to the artificially induced perturbation.

The response is fundamentally different for a convecting fluid system than it is for an exclusively solid rock conductor. A full three-dimensional analysis of the thermal perturbation problem allows calculation of the local fluid velocity vector and a good resolution between convective and conductive heat flow. The new probe has been successfully tested recently under field conditions at Long Valley, California, a thermally active potential target area for the Continental Scientific Drilling Program.

(Sandia National Laboratory at Albuquerque, J. Dunn)

17. Neutron "Time-of-Flight" Techniques Measure Residual Stresses in Structural Materials

Neutron "time-of-flight" techniques have been used to successfully measure residual stresses in cermet materials and in a zirconium alloy. The information on cermet materials is important in the design and development of drilling inserts for oil and gas well drilling apparatus. The detailed information on residual stresses in the zirconium alloy provides valuable data for reactor fuel element and pressure tube design and performance analysis. This new non-destructive method for measuring internal residual stresses in structural alloys was developed using neutron time-of-flight measurements and its success depends critically on the high resolution powder diffractometer located at the Intense Pulsed Neutron Source at Argonne. The technique was first applied to examine the zirconium alloy tubing used as fuel cladding in water reactors. It was demonstrated that it suffers from residual tensile stresses in the circumferential direction and compression through the thickness; this combination can lead to unexpected and unacceptable creep of the cladding in service. The second application was to measure the stress level in the metallic binder phase of a hard ceramic-metal composite used as drill bit inserts for rock drilling; the high tensile residual stress found can cause premature failure of the drill bit.

This research has developed and applied a non-destructive method for characterizing quantitatively internal residual stresses. No other probe has been successful in achieving this, with the possible exception of an acoustic technique. This research will impact technically on the processing of structural materials, namely, to change these to reduce unwanted stresses and enhance desired ones. The potential economic impact is large in terms of allowing improved reactor fuel utilization in the case of the zirconium alloy and longer drill-bit life in the case of the composite noted above.

(Argonne National Laboratory, J. Faber, in collaboration with Chalk River Nuclear Laboratory, Canada,

18. Helium Atoms Found to Create Lattice Defects in Metals

A new physical process by which an impurity (helium) can produce lattice damage in metals in the absence of externally-supplied energy (i.e., thermal, radiation) has been verified experimentally. It has been known for some time that helium atoms are readily trapped in metals that have large numbers of defects in their lattice structure, e.g., as in damaged metals. More recent research has shown that helium atoms also become strongly trapped in metals with low intrinsic defect concentrations. These results stimulated calculation of lattice defects to account for the observations and have led to a model involving self-trapping of the helium. This theoretical work was followed by microscopic verification of helium-induced bubble formation in tritium charged palladium and in gold where helium was implanted at energies below the threshold that would normally cause lattice damage. In addition, evidence of helium-induced bubble formation has been found in vanadium and niobium. These latest studies have yielded new data on bubble growth processes and helium-dislocation interactions.

Thus the process of helium self-trapping in metals whereby helium forms its own lattice defects which nucleate helium gas bubbles was first indirectly inferred from experiment, then predicted by theory, and finally experimentally confirmed for four different metals and metal hydrides.

These results alter present thinking on the role radiation damage plays in helium bubble formation in metals and have shown that helium-induced degradation of metals cannot be ruled out as a potential problem area in long-term fusion energy applications. They also call attention to the possibility of future materials problems in all nuclear-based technologies. These results are directly applicable to other ongoing modelling studies of material response in fission reactor environments.

(Sandia National Laboratories-Livermore, W. D. Wilson, G. J. Thomas, and M. I. Baskes)

19. New Method to Uniformly Blend Ceramic Powders With Sintering Additives Improves Properties

A new method was developed for the homogeneous addition of sintering aids to silicon nitride powders. Sub-micron sized silicon nitride powder, when sintered, or heated under defined conditions, becomes a high-temperature structural ceramic. Sintering aids promote this process. Homogeneity of the unsintered compacts is an essential requirement in order to properly sinter silicon nitride to obtain uniform, reliable, ceramic components. The method developed is based based on the use of colloidal dispersion forces, first, to break down and prevent the formation of agglomerates in unsintered compacts of silicon nitride powder, and second, to promote mixing by causing uniform dispersion of sub-micron powder mixtures of silicon nitride and the sintering aids yttrium oxide and magnesium oxide.

A comparison of the mixing achieved by this new process with that achieved by conventional powder processing routes showed that this new method provided a dramatic improvement in the uniformity of silicon nitride unsintered compacts.

Homogeneity of the unsintered compacts containing silicon nitride and its sintering aids is necessary to produce a homogeneous flaw-free microstructure by the sintering process. Such a microstructure is required if the silicon nitride is to have good mechanical properties at 1500°C, such as for potential use in advanced turbine blades.

(Rockwell International Science Center, F. F. Lange and T. M. Shaw)

20. New Method Devised for Monitoring Thermally Enhanced Oil Recovery

The velocity and attenuation of seismic waves traveling through rocks is strongly influenced by the properties and spatial distribution of the pore fluids present. An investigation of these phenomena and their relation to bulk rock properties, pore distribution in the rock, and the presence and nature of the pore fluid, has led to a new method for reliable remote monitoring of the progress of steam flooding and other oil recovery methods. The advance results from the ability to follow changing oil temperature throughout the process. While measuring the velocity and amplitude of seismic signals as a function of pressure (up to 200 bars) and temperature (up to 150° degrees C), very large reductions in velocity (50%) and wave amplitude (7 fold) were detected when heavy-oil saturated sandstones were heated under *in situ* pressure conditions.

Making use of this effect, an array of seismic receivers and transmitters deployed over an oil reservoir can be used to monitor the progress of a thermal oil recovery operation. The array measures the variation of seismic velocities and amplitudes during the recovery operation, and these data can, in turn, be used to model changing oil temperature throughout the reservoir.

(Stanford University, A. Nur)

21. Improved Method Developed to Describe Crack Strain Fields in Heavy Piping and Pressure Vessels

An effective computational method was developed which permits far more realistic properties of materials to be employed in the design of major components of energy plants than allowed by current design codes. The new method which is a finite element technique, treats the deformation behavior of metals in a manner termed "incompressible-fully plastic." Though still an approximation, this is far superior to previous descriptions of strain fields around cracks in piping and pressure vessel alloys where the materials were treated as "linear elastic."

With the new finite element technique, engineering calculations of the stability of a crack have been carried out under the auspices of the Electric Power Research Institute. It recently published a handbook as a reference source for solution of crack stability problems in piping and pressure vessels, which acknowledges that the calculations were made possible by the development of this finite element technique.

By providing a computational method for accurate failure analysis, this research has paved the way for proposing improved design criteria for qualifying structural components in nuclear reactors with lower initial cost than with current codes. The improved design criteria will also assist in qualifying components for continued service; the economic value of this is significant as well, given given the current trend toward extending utilization of existing plants rather than building new ones.

(Brown University, R. Asaro, J. Gurland, and A. Needleman)

22. Miniaturized Thermionic Elements Introduced into Integrated Circuits

Measurements of temperature, pressure, mass flow rates and the like often have to be carried out in an envirommment in which the usual instrumentation fails. Devices using semiconductors, for example, cannot be employed at temperatures above a few hundred degrees. On the other hand, devices using electron emitting elements (as in the triodes of vacuum tubes) can in principle operate well in a variety of hostile environments, but until now no way had been found to incorporate such elements in integrated circuits comparable to semiconductor microcircuits.

Recently a promising step toward solving these problems has been completed. Extremely small thermionic elements have been devised and shown to be well adapted to fabrication and use in microcircuits etched on silicon chips. Packing densities of 1000 circuit elements per square inch have been achieved and outstanding tolerance of high temperatures and radiation levels has been demonstrated. The present state of this art is not yet at its limits and further important advances are anticipated.

Unexpectedly, early results from this research have attracted the attention of a major computer products manufacturer and are being applied by that manufacturer to computer terminal display tubes. The tubes will feature an electron gun with multiple sources and built-in capability for signal processing. Although this application was not foreseen, a broad range of applications of the new integrated thermionic circuit technology is expected in the long run for instruments of interest to DOE energy and defense programs.

(Los Alamos National Laboratory, B. McCormick)

23. Unexpectedly Fast Electron Transfer Across Large Molecules Discovered

A novel set of experiments has demonstrated that electrons move surprisingly fast across large molecules. The molecules were designed with a rigid bridge separating parts of the molecule that can accept electrons at fixed, known distances. In the experiment electrons generated in a linear accelerator attach themselves at one end of each molecule and the rate at which they move to the other end is measured. Because the measured rates are extremely fast, and the spacer region is an electron insulator, it was determined electron transfer was accomplished by a "tunneling" or jumping mechanism. These results are of particular importance in the solar photochemistry research area where initial charge separation following absorption of light energy may be accomplished following such a jump.

(Argonne National Laboratory, J. Miller)

24. Neutron Reaction Cross Sections Extended By New Technique

High resolution measurements of neutron and gamma ray production cross sections have been made for the first time for neutron bombardment energies above 15 MeV. These measurements were made simultaneously over the range from 200 keV to 40 MeV using the intense pulsed beam time-of-flight system at the Oak Ridge Electron Linear Accelerator (ORELA) and were made possible by a new technique based on a high resolution lithium-doped germanium detector. Although these cross sections are of primary interest to the Office of Fusion Energy, the initial measurement provided information of timely importance to the fast reactor program, clearing up a troublesome descrepancy between experimental and theoretical results for an important design benchmark, the "large iron sphere". The measurement of the isotope iron-57 demonstrated that this minor component of natural iron (2.2% abundance) can not be ignored in the calculation. The observation of a surprisingly intense gamma-ray line, the measurement of which was made possible by the high resolution detector used, also has provided valuable information for the theorists who are developing a complicated nuclear model for the calculation of these cross sections.

The cross sections being measured with the new system are of interest not only for direct input into calculations of neutron transport and activation, but are also contributing to the development of a computational model that will permit the prediction of cross sections for high energy neutron reactions that are difficult or time-consuming to measure, but are needed for inclusion in the Evaluated Nuclear Data File (ENDF) maintained by DOE.

(Oak Ridge National Laboratory, D. Larson)

25. Elusive Energy Loss Process Affecting Fusion Verified

Measurements of dielectronic recombination, a process that has eluded experimenters for years, have finally been made. The dielectronic recombination cross sections for the doubly charged ion of boron were measured; that is the first time such measurements have been made for an ion with multiple charges

Dielectronic recombination involves the loss of energy in a plasma and occurs when energy is absorbed by an ion when it captures an electron in the plasma. At the instant of capture, the positive charge on the ion is reduced by one unit and the resulting ion is left with excess energy. The ion next rids itself of the extra energy by the release of a photon most likely in the form of an x-ray. The net effect of all this is that the energy initially provided to effect a collision between two atoms and cause fusion of the two nuclei is instead lost through radiation. The process is important to the understanding of the behavior of plasmas and its measurement helps provide a more accurate account of the energy balance in a fusion plasma. This account in turn will permit the improved design of efficient fusion power plants.

The existence of the process was first suggested in the 1940's to account for observations made by astrophysicists to explain energy balance in stars. They could only observe the sum of several simultaneous processes, of which dielectronic recombination was one. Experimental study of the single isolated process was not possible. Now the process has been demonstrated by directing a beam of ions from an accelerator into a specially designed chamber filled with electrons. Close inspection of the interaction taking place in the chamber between the ions and electrons showed the effect sought.

While the first results are in some disagreement with theory, the fact that the process can now be studied experimentally is clearly a breakthrough in the field of high energy atomic physics and a significant contribution to our improved understanding of fusion plasma interactions.

(Oak Ridge National Laboratory, S. Datz, & co-workers)

26. Transposition of Genes in Higher Organisms Quantified for the First Time

Only recently has it been appreciated that genetic transposition (movable genes) does occur in a broad range of organisms. This phemonenon, which was discovered in maize by Dr. Barbara McClintock about thirty years ago, has never been quantified as to its rate of occurrence.

In a specially designed genetic system in maize the frequency of transposition of genes associated with the restoration of male fertility has been measured. This represents the first time that these events of movement of genes have been put on a numerical basis. Such results will assist in assessing the importance of genetic transposition and in understanding the phenomenon itself.

(University of Illinois, J. Laughnan)

27. New Method for Numerical Solution of Turbulent Combustion Model

Difficult questions in computational mathematics arising from the need to simulate real problems are being examined. One such question is a fundamental and complex problem in the area of turbulent combustion: the analysis of the effect of turbulence on the propagation of a flame. At high Reynolds number, turbulent eddies and recirculation zones form due to viscous effects. This affects the position of the flame and the distribution of unburnt fuel available for combustion. This interaction is of great importance in the design of internal combustion engines. The problem is to discover how to direct the flow in such a way that the largest amount of fuel is burned as quickly as possible, thus maximizing the force on the piston and minimizing the amount of unburnt fuel expelled at the end of a stoke.

To investigate these phenomena, a numerical technique was developed to approximate the solution of a mathematical model of turbulent combustion. This technique is specifically designed for flow at high Reynolds numbers. It portrays in a natural and effective manner the development of turbulent eddies and recirculation zones in the flow. The motion of the flame is handled in a manner that avoids the instabilities and inaccuracies that plague other front tracking techniques. The results of "numerical" experiments with this new technique on turbulent combustion in open and closed chambers show the effect of heat-producing reactions and viscosity on the rate of combustion. Heating effects along the front are seen to increase the speed at which the flame travels through the domain, decreasing the amount of time required for complete conversion of reactants to products. Viscous effects, on the other hand, both retard and accelerate flame advancement. Although the turbulent eddies produced by boundary conditions inhibit burning in corners and near walls, they also "wrinkle" the flame, increasing the surface area available for combustion. These "numerical" experiments represent a major step towards understanding the combustion process.

(Lawrence Berkeley Laboratory, J. Sethian, A. Chorin)

28. Unexpected Photochemical Mechanism Discovered in Enzyme Process for Biomass Hydrogen Production

A new photochemical route to the utilization of photons for enzymatic dissociation of water to produce hydrogen from biomass has been discovered. Experimental measurements of the simultaneous generation of hydrogen *and* oxygen by a laser light saturation technique have established the unexpected insight that not all photodissociation of water occurs by the same photochemical mechanism. By examining the hydrogen to oxygen ratio, it was apparent that the rate of hydrogen and oxygen generation was inconsistent with the time-accepted Z-scheme mechanism of photosynthesis. The hydrogen to oxygen ratio was found to be significantly below the 2:1 ratio of water's composition, which suggested the existence of a chemical step that encumbers the release of hydrogen. The fact that a previously unexpected mechanism exists for the enzymatic dissociation of water in biomass systems has broad implications for future developments in solar photochemistry as well as in the case of biomass photolysis.

(Oak Ridge National Laboratory, E. Greenbaum)

29. Physics Model Computations Nearly Ten Times Faster Using New Computer With Parallel Architecture

Techniques for accelerating execution of practical computational problems by using parallel processing techniques on an experimental computer have been successfully demonstrated. In mid-1983, a Denelcor HEP-1 computer was acquired as part of the DOE activity in experimental parallel architecture research.

Three problems common to the DOE activities in computational modeling were addressed: a particle-in-cell model, commonly used in plasma physics models; a hydrodynamics model, used in weapons design and combustion modeling; and a Monte Carlo model, used in modeling critical phenomena in materials and in fundamental particle physics. In each case, the problem was studied with the aim of redesigning the algorithms into sets of independent processes that could be executed concurrently. The HEP-1 architecture provides a mechanism for simultaneously executing a large number of independent processes, thereby speeding up the computation by a factor proportional to the number of processes. It was demonstrated that the computations involved in each of these modeling problems could be carried out about ten times facter with this architecture.

These results hold great promise for the design of even faster parallel architecture computers for large scale scientific computation.

(Los Alamos National Laboratory, B. Buzbee)

30. Genes Controlling the Primary Events of Photosynthesis Identified

Using molecular genetic techniques scientists have succeeded in cloning and sequencing of the nucleic acids of five genes which code for some of the first steps in photosynthesis. This work represents the first time that it has been possible to precisely locate specific genes that code for proteins involved in the primary events of photosynthesis in a structure known as a reaction center and the related "light harvesting" pigment area. This work was done with the photosynthetic bacterium known as Rhodopseudomonas capsulata; however, similar genes are operative in higher plants. Further, the region of common function in this genetic material has been conserved over three billion years, the estimated evolutionary time between the bacteria and higher plants.

The significance of the work is that it permits more incisive questions to be asked about the structure and function of the biological energy conversion entity known as the photosynthetic apparatus. For example, the information on the nucleic acid sequences is easily translated in amino acid sequences in the photosynthetic proteins. That information has led to clues about how some of the components of electron transport (quinones) are attached to the proteins.

In addition, some of the proteins also have homology with those that are involved in the action of some widely used herbicides in crop production. Thus such information may also provide leads into understanding of herbicide action and possible strategy for better molecular designs of herbicides.

(Lawrence Berkeley Laboratory, J. Hearst, and K. Sauer)

31. New Techniques Developed for Analyzing Near-Surface Reactions

Two new techniques, one involving electron and photon desorption, and the other pulsed laser field evaporation have provided the means to substantially advance the understanding of atomic and molecular motion in the near surface regions of solids.

Photon stimulated desorption studies of cleaned silicon surfaces revealed that hydrogen migrating from the bulk to the surface displays a complex surface reaction resulting in the formation of hydride phases. These studies are important not only for the determination of bonding site, electronic state, and geometric configuration, but also to the technological goal of removing hydrogen from silicon.

Pulsed laser studies have shown that surface crystallography plays a major role in the catalytically important process of molecular dissociation. The temperature range over which carbon monoxide molecules dissociate has been measured, as has, for the first time, the activation energy between flat and stepped regions on the surfaces of molybdenum. These experiments showed that highly-charged field-evaporated ions are formed away from the surface after the atom has desorbed to a lower charge state.

The advances in both of the techniques will permit new insight into surface and near-surface reactions which are important to a number of technological areas.

(Sandia National Laboratory - Albuquerque, M. Knotek and G. Kellogg)

32. Dose Dependence for Defect Production Mechanism Found Using ANL High Voltage Electron Microscope (HVEM)

The unique capabilities of the Argonne National Laboratory High Voltage Electron Microscope/Tandem van de Graaff have recently been employed in attacking a controversial issue involving the nature of defects formed in the alpha-phase of iron during neutron irradiation. The basic character of the defect structure produced during neutron irradiation was reproduced by ion bonbardment and examined in situ at 40°K in the ANL-HVEM. The defect formation mechanism observed differs from what had been assumed previously, and is different from that for most other metals. It was found that the defect producing mechanism caused by high energy knock-ons (in either ion or fast neutron irradiation) changes when the dose is high enough. This research, uniquely dependent on the ANL-HVEM capability, is the first demonstration of a dose dependent change in a defect production mechanism. It will have to be included in valid models of irradiation behavior in the future and could have important consequences for predictions of radiation damage in iron and ferritic alloys. The low swelling character of these materials may, in part, be related to this newly discovered effect.

(Argonne National Laboratory, M. Kirk, and University of Illionis, I. Robertson)

Mrs. SCHNEIDER. That would be great. We appreciate it. I have had the opportunity, but not from DOE, to get information on some of the latest technological fixes in the manufacturing process, and I brought experts to the State of Rhode Island, to the manufacturers who were on the brink of closure, and said, "Look, you can recycle your waste heat, and you can do this, and you can do that." That was great. I felt that I was providing a public service. I am wondering how much more of that kind of information is out there that I will never know about unless I ask, and my constituents will never have the benefit of unless I ask. So I am open and receptive to any solutions to energy efficiency that you may have.

Mr. LEWIS. Thank you, Mrs. Schneider. Thank you, Dr. Trivelpiece and Dr. Kropschot.

Mr. FUQUA. Our next witness is Prof. George Pimental, associate director, Chemical Biodynamics Division, Lawrence Berkeley Laboratory.

Thank you very much for being here. We always appreciate having you.

STATEMENT OF DR. GEORGE C. PIMENTEL, PROFESSOR OF CHEMISTRY, UNIVERSITY OF CALIFORNIA, CHAIRMAN, NAS/NRC COMMITTEE TO SURVEY THE CHEMICAL SCIENCE; DIRECTOR, LABORATORY OF CHEMICAL BIODYNAMICS

Dr. PIMENTEL. I want to thank the committee for letting me speak to you today about the initial conclusions of the NAS, NRC committee to survey the chemical sciences. I have submitted written testimony, and I would like to summarize it.

Mr. FUQUA. Yes, we will make the written statement part of the record. If you wish to summarize, please go right ahead.

Dr. PIMENTEL. The initial conclusions I mentioned are embodied in the briefing report, which is part of that testimony. This briefing report was orally presented to OSTP in the various agencies, including Department of Energy, last October.

We have examined the state of chemistry today, its special opportunities, and the benefits these opportunities might bring to our society. As I speak, I want you to know that I feel I am representing consensus views of the entire chemistry community, since we have had contributions from over 200 of this country's most creative chemists, each reporting on the frontiers opening in their own specialty area. This collection of essays proves that this is indisputably a time of rich opportunity in chemistry.

A prime reason for this is the development of powerful instrumental probes that permit chemists to address fundamental questions that were simply beyond our measurement and calculational limits only a decade ago. These new capabilities and the priority areas they define are of direct applicability to the mission goals that justify the DOE research program.

First, I would like to try to convince you that chemistry is a central science that is especially important in responding to society's needs. Prima facie evidence is found just in the composition of the scientific workforce of this country. Our industries employ 87,000 chemists, 64,000 chemical engineers. That is a total of 150,000 chemistry professionals. For a comparative scale, U.S. industry hires 37,000 biological scientists and 22,000 physicists.

An industry remains alive only if it has products and processes that are demonstrably valuable to society. An industry hires each professional deliberately to maximize their response to the needs of the public. Industry decides 150,000 chemists and chemical engineers, 37,000 biological scientists, 22,000 physicists. What about the Department of Energy?

The mission of the department must be to guarantee for the rest of this century and beyond continued access to abundant but also clean sources of energy. Its research programs must look ahead to provide the fundamental base of knowledge that will be needed by industry as it builds the energy technologies of the future. Looking ahead two or three decades, it is easy to see that the strength of the DOE chemistry programs will be the key. Today, about 92 percent of the U.S. energy supply is derived from fossil fuels—petroleum, gas, and coal. Next, at about 4 percent, is hydroelectric, but this percent is not increasing because of environmental concerns. Third, is nuclear, at about 3.5 percent, but again that may not increase much because of social concerns. Who really knows when or whether fusion energy might become a reality; perhaps well into the first half of the 21st century.

So, for the next two or three decades, we will be looking for chemistry based new energy sources, the ones you were asking about. I say "new" because we are running out of the easy ones. Already 80 percent of the known and recoverable U.S. supply of crude oil has already been extracted and consumed. Already coal use is rising relative to petroleum, a trend that is going to continue as world production in petroleum peaks out around the turn of the century and begins its inevitable decline.

We must be looking to new sources, unfortunately: lower grades of crude oil, coal, shale, tar sands, and lignite. Let me consider lower grades of crude oil. That means different chemical compounds than we are used to refining, with more impurities like sulphur, gives us acid rain, and catalyst-killing metal impurities, like vanadium. All of that means new processes. The same difficult story applies for lower grades of coal, for shale, for tar sands. Perhaps we will find ways to use biomass efficiently and economically. That is a research area that we must pursue. Perhaps we will learn to harness photons—that is, solar energy—through photochemistry, photo-electro-chemistry, and photovoltaics. In all of these, chemistry will be the lead science in the energy sources of the immediate decades ahead.

This Federal agency, the Department of Energy, might as well carry a pseudonym. It is the chemistry agency.

Let me talk about combustion. We spend 10 percent of our GNP on combustion materials. Only a 5-percent increase in the efficiency with which we burn coal, oil, and gas would be worth an estimated $15 billion a year to our economy. The value would be absolutely immeasurable, if at the same time we could eliminate, as we absolutely must, air pollution, acid rain, and global carbon dioxide accumulation.

You might wonder, how can we learn more about combustion? This is a technology as old as the discovery of fire. Well, surprisingly, there is no subarea of chemistry offering greater promise. With lasers and computers in their hands, chemists are making amazing advances in our knowledge of what controls the speed of a chemical reaction. We can now track chemical changes that take place in a millionth of a millionth of second. We can now detect crucial transient molecules that are present at parts-per-billion levels. With these new instrumental probes, we can now dissect and understand the anatomy of a flame. We can write the biography of an explosion.

What about these new energy sources we were talking about? Cannot we leave it to industry to solve the complex chemical and environmental problems they will bring? Is there a legitimate and appropriate role here for federally supported DOE research programs? I answer, There certainly is. The answer to many of the foreseeable problems will lie, for instance, in the design of better catalysts. But only over the last decade has catalysis begun moving from an empirical art toward becoming a science.

A fundamental base of knowledge is what is needed. For example, rational design of soluble catalysts can be seen to be on the horizon because of remarkable progress in the synthesis of organometallic compounds. This progress relies on sophisticated instrumentation with intimidating names, like Fourier-Transform nuclear magnetic resonance, computer-controlled X-ray spectroscopy, tandem mass spectroscopy. These are essential instruments, and unfortunately they also have intimidating price tags. Each one might cost several hundred thousand dollars.

With them, we can remain in our world leadership position in the design of next-generation soluble catalysts. Without these instruments in the hands of our research scientists, we can look ahead to U.S. industries buying patent rights from Germany, Japan, and France.

Equally exciting and immediately relevant to your committee's interest in new materials are the advances now coming in solid-state catalysts. A virtual explosion of new instrumental techniques has appeared over the last 15 years to give us at last experimental access to this two-dimensional reaction domain. Now that chemists can see what molecular structures exist on the surface, all of our knowledge of reactions in conventional settings becomes applicable. Again, these marvelously sensitive instrumental probes are expensive. As more chemists are able to purchase them, chemistry on surfaces will come under intensive study, and the cornucopia of new catalysts will open.

The promise of the field of catalysis has been recognized abroad, you can expect. In particular, in the U.S.S.R., Japan, Germany, and France. To stay in the vanguard in this field, we must enhance the vitality of our own chemical catalysis research programs, including those sponsored by DOE.

Now let me speak about materials. This desk top is a material. My shirt is a material. The heat shield on a spacecraft is another. All of the substances out of which one could construct autos and airplanes, bridges and buildings, tires and transistors, windows and walls, those are all materials. The next two decades are going to bring many changes in the materials of our daily lives.

Let me give you this example. Metals are going to be used sparingly, as tailored materials outperform them in many of their traditional functions. What do I mean by tailoring? Let us consider this molecule here. That is polymethylacetylene. It is a member of a family of organic polymers that, on suitable chemical treatment, become electrical conductors almost as good as copper.

I have indicated by these little black appendages here some added parts. That is to signify to you that from this starting point, an organic material that conducts electricity as good as copper, a chemist can add other desired properties. He can tailor it to need. Do you want it green? soft? hard? to soften on warming? to get hard on warming? magnetic? fluorescent? to stick to glass? to bond to silicon? to repel water? be biodegradable? photodegradable? you name it? Do you want it in threads, films? any combination? Whatever you want, fill in the blanks. All of those are within our grasp through chemical research.

Ultimately, the control of the properties of any material depends on understanding its composition, bonding, and geometry at the atomic molecular level. That is the chemist's home territory. What we can do with this understanding then depends on what we can make, and synthesis is again the chemist's bag.

I could give a catalog of new materials and the new incentive for chemical synthesis they awaken that is much longer than time permits. I will just mention a few. The polymer, which has the trade name Kevlar, has a tensile strength-to-weight ratio 6 times higher than that of drawn steel, 10 times higher than that of aluminium. No wonder it is flying around the country as a major structural component in hundreds of commercial airliners. It provides an answer, Congresswoman Schneider, to your question about examples of where energy is being saved. Every one of these airliners has a tail section of Kevlar that saves about 2 million gallons of fuel over the lifetime of the aircraft because of the reduction in weight. That, of course, came from organic synthetic chemistry.

Another example. New families of organic conductors called metallo-macrocycles have been synthesized, in which large flat molecules are chemically laced together in a stack to hold the charge-transfer units in a predetermined and rigidly enforced geometry. Another example: a 1,000-speed color film, based on crystal defects to control crystal growth. Liquid crystal devices based on molecules, deliberately structured with preplanned charge distribution and shape. Organic photoresist polymers, suitably sensitive to electron beams, X-rays, or ultraviolet light for microchip fabrication. Materials for extreme conditions—jet engine and automobile engine parts, nuclear and fusion reactor components, and spacecraft heat shields.

And let me end with the ultimate challenge to the chemist, to synthesize molecular scale memory chips. These are exciting prospects that are attracting more and more chemists to the materials sciences. This is a trend DOE should encourage and accelerate. The chemist's talents are not the only ones needed, but they are among the essential ones.

So where does all this lead? It seems clear that the present state of excitement and opportunity in chemistry can and should be exploited to advantage by DOE in pursuit of its energy-oriented mission. So it leads me to look at the Department of Energy research budget and compare its program levels to the careful considerations made by the briefing panel concerning the investment needed to take advantage of the exciting prospects ahead.

The briefing panel became convinced that these opportunities warranted an immediate infusion of $50 million real growth into the relevant NSF and DOE programs in chemistry, the subject area I talked about today. According to my reading of the President's budget, the DOE energy science program proposes in fiscal year 1985 combined operations and capital equipment, which includes instrumentation and, I take it, also some fixing the roads, a budget of $89.7 million. This provides a net increase of $7.7 million for a 9.4-percent rise that must take up inflation. This amount should be increased by $10 million to $99.7 million. The increment should be divided between operations and scientific instrumentation to favor instrumentation.

The DOE materials science program, combining operations and capital equipment, has a proposed fiscal year 1985 budget of $157 million. This is a net increase over fiscal year 1984 by $19.1 million, a 13.9-percent rise. This amount should be increased by $5 million to $162 million. Both of these added increments should be focused on stimulation and support of the priority research areas described in the briefing report; that is, understanding chemical reactivity and catalysis as they apply to the energy mission of DOE.

I want to thank you again for letting me tell you about the briefing report and its relevance to the DOE programs you are considering today and the opportunities that are before us. I would be pleased to answer any questions about the chemical survey or about the testimony I have presented today.

[The prepared statement of Dr. Pimentel follows:]

TESTIMONY OF

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Chairman, Committee to Survey Opportunities
in the Chemical Sciences
National Research Council

It is appropriate to your purposes today to hear of the initial conclusions of the NAS/NRC Committee to Survey the Chemical Sciences. These conclusions are embodied in the Briefing Report (included herewith) that was orally presented to OSTP, OMB, and the various Agencies, including DoE, last October. The report reveals a time of exceptional opportunity in chemistry today, and many of these opportunities relate to the mission goals that justify the DoE research programs.

The Chemistry Survey Committee is formulating a multiyear program to exploit the richest potentialities. We have identified three priority areas that will yield the greatest rewards; they furnish the appropriate beginning to that program.

A. Understanding Chemical Reactivity

B. Chemical Catalysis

C. Chemistry of Life Processes

The first two of these priority areas are immediately relevant to the mission of the Department of Energy. Substantial real growth in them is needed; it would be a wise investment in the future of our country. The existing excellent NSF and DoE Chemical Sciences and Materials Sciences programs are the proper locale for this growth.

CHEMISTRY AND THE DOE MISSION

Chemistry is a central science that is especially important in responding to societal needs. This is evident in the simple statistics that US industries employ 86,600 chemists and 63,700 chemical engineers, a total of 150,000 chemistry professionals. For comparison, US industries employ 37,400 biological scientists and 22,400 physicists.* More specifically, chemistry is of predominant importance in the energy technologies that keep the wheels of our industrial society turning, that are responsible for the richness of our culture and our economic success in world markets. Again, de facto proof of this dominant role of chemistry is contained in simple facts about the nation's energy sources. In 1980, fossil fuels furnished more than 92% of US energy use, to be compared to 4% by hydroelectric and 3.5% for nuclear.** This balance will not noticably change due to the growth of either hydroelectric or nuclear energy in the coming decades. As for fusion energy, even optimistic proponents are reticent to predict that it will become our leading energy source in less than forty years. No, the present overwhelming dependence upon chemistry-based energy technologies will certainly persist for the rest of this century and undoubtedly well beyond. Yet, no single factor is more critical to the long-term health of our technological society than continued access to abundant and clean sources of energy. The prime mission of the Department of Energy research program must be to guarentee this access. The strength of its chemistry programs will be key in DoE's fulfillment of this critical responsibility.

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* "US Scientists and Engineers 1980" NSF 82-314, NSF 82-305
** Petroleum, 45%; gas, 27%; coal, 20%. "Statistical Abstract of the United States, 1982-83," U.S. Dept. of Commerce, Wash.,D.C. 1982

ENERGY SOURCES IN THE YEAR 2000

Why speak of energy sources at a time when there is an oil surplus? It is because DoE's research programs must have long-range horizons - they are aimed primarily at protecting the long-range interests of our society. They must not be distracted from sure problems of the future by day-to-day fluctuations. To illustrate, between 1978 and 1980, US petroleum consumption dropped 10% but in the same two year period, coal consumption rose 11.5%. This trend is likely to become familiar. Twelve percent of the world's known oil supply has been discovered in the US, one third of which is classified as recoverable by present extraction methods. It is sobering to realize that 80% of the US-recoverable supply has already been extracted and consumed!

So where will the US energy be coming from in the year 2000? It won't be fusion nor is it likely to be mostly nuclear. Petroleum and gas will still be important, though we will be increasingly dependent on foreign supplies and their world production will have peaked and begun their inevitable decline. We must be looking to new sources: lower grades of crude oil and coal, shale, tar sands, biomass, and solar. But in every one of these forseeable alternatives, important developments are needed in which chemistry and chemical engineering play a dominant role. The fundamental nature of the needed advances dictate an immediate commitment to a strengthened DoE research program in chemistry. This program can exploit the powerful array of new instrumental methods that promise rapid advances on each of these critical frontiers.

1. Combustion processes
2. Catalysis and chemical reactions on surfaces
3. New materials for new technologies

4. Chemical and electrical storage of solar energy

5. Environmental protection with new energy technologies.

I will speak further on the first three of these frontiers.

COMBUSTION

The US currently spends 10% of its GNP on combustion materials. An increase of only 5% in the efficiency with which we combust coal, oil, and gas would be worth an estimated fifteen billion dollars per year to the US economy. The gain would have immeasurable additional value if it is accompanied (as it must be) by reduction in air pollution, acid rain, and global CO_2 accumulation.

How can we learn more about a technology as old as the discovery of fire? Surprisingly, there is no subarea of chemistry offering greater promise. Because of powerful new instrumental tools, lasers and computers leading the way, chemists are making amazing advances in our knowledge of the speed of chemical reactions. This is a prime basis for our priority thrust A, Understanding Chemical Reactivity.

To be explicit, in the past, limits to complete understanding of the temporal aspects of chemical change arose from our inability to detect transient molecular species that are of critical importance at extremely low concentrations in flames and explosions. Furthermore, these elusive intermediates engage in transient chemical events that have been too rapid to be tracked. Now lasers have essentially removed both obstacles. Chemists can now interrogate a reacting mixture on a time scale as short as a millionth of a millionth of a second (a "picosecond"). This means we can hope to measure the lifetime of any molecular species that can be said to have an identifiable molecular identity. At the same time, lasers have extended detection limits downward by as much as six orders of magnitude below that possible fifteen years ago. Suddenly we have the capacity to dissect and understand the anatomy of a flame. All that is needed is wider access to the sophisticated (and expensive) instrumentation that gives us these remarkable probes.

CATALYSIS

It has been estimated that 20% of the GNP is generated through the use of catalysis in satisfying a wide range of societal needs, including energy conversion and environmental protection.

Two remarkable examples of catalysis chemistry to the rescue are provided by lead-free gasoline and the catalytic auto exhaust. Platinum-iridium solid state catalysts are responsible for our ability to "reform" unbranched hydrocarbons into high octane fuels that eliminate need for tetraethyl lead. It is easy to take such an industrial feat for granted, though it involves chemistry of perilously flammable substances handled on a gargantuan scale. Suffice it to say that use of lead-free gas in Europe is being held back because a number of countries, including France, do not yet have production and distribution capabilities in place. The other example is equally gratifying. Every car running on lead-free gas has about two grams (less than one tenth of an ounce) of a platinum-palladium-rhodium catalyst in its exhaust system to oxidize unburned hydrocarbons and carbon monoxide to harmless water and carbon dioxide.

A catalyst accelerates a chemical reaction without being consumed. Recent research innovations over the last ten years are converting catalysis from an art to a science. Rational design of soluble catalysts is now within the realm of possibility because of exciting progress in the synthesis of organometallic compounds. Catalysts can even be made to produce only one of two possible mirror-image related molecules. For example, L-dopa is an amino acid that has revolutionized treatment of Parkinson's disease. Now we have a soluble rhodium phosphine catalyst that produces the desired active structure in 96% yield, virtually eliminating the inactive mirror image counterpart. Perhaps more obviously connected to DoE interests, soluble organometallic compounds will undoubtedly figure in our increasing dependence upon synthesis gas (carbon monoxide and hydrogen) produced from coal as a source of chemical feedstocks.

What accounts for the acceleration of progress in metalloorganic chemistry? Again, sophisticated and expensive instrumentation is a crucial element. Nuclear magnetic resonance and mass spectra show rapidly and reliably what elements are present in a new compound and their structural environment. Then x-ray crystal structure analysis reveals the precise molecular structure. Progress is strongly determined by access to this powerful instrumentation.

Equally exciting and immediately relevant to your Committee's interest in new materials are the advances now coming in heterogeneous catalysis. These are solid state materials prepared with large surface areas upon which chemical reactions can occur at extremely high rate and selectivity. A virtual explosion of new instrumental techniques has appeared over the last fifteen years to give us, at last, experimental access to this two-dimensional reaction domain. Now that chemists can "see" what molecular structures exist on the surface, all of our knowledge of reactions in conventional settings becomes applicable. As more chemists are able to purchase the instrumental probes, chemistry on surfaces will come under intensive study and will surely result in a cornucopia of new catalysts.

The promise of the field of catalysis has been recognized abroad, in particular, in Japan, Germany, the USSR, and France. To stay in the van in this field, we must enhance the vitality of our own chemical catalysis research programs, including those sponsored by DoE.

NEW MATERIALS FOR NEW TECHNOLOGIES

The next two decades will bring many changes in the materials in which we are clothed, housed, and transported, the materials of our daily lives. New industries will be founded - as polymers led to synthetic fabrics, as phosphors led to television, as semiconductors led to computers. Metals will be used sparingly as tailored materials outperform them in many of their traditional functions. It is the potentiality for tailoring that points to the increasing role for chemists in this interdisciplinary field. Ultimately the control of the properties of any material depends upon understanding its composition, bonding, and geometry at the atomic/molecular level - the chemist's home territory. What we can do with this understanding then depends on what we can make - and synthesis is again the chemist's bag.

The zeolites furnish an appropriate first example. These are remarkably effective catalysts for a variety of reactions, including "cracking" high molecular weight crude oils to volatile, high octane fuels. Zeolites are crystalline alumina-silicates that chemists now synthesize with cavities and channels deliberately shaped to accommodate particular reactants and products. Guest molecules that slip comfortably into these channels can be held in favored conformations as reactants bring about desired chemical changes. The zeolites present prototypes for entirely new solid catalyst systems.

In the polymer field, there are many exciting frontiers. The potentiality of polymers as structural materials is expressed vividly in the hundreds of commercial airplanes flying today that have substantial structural elements made of an organic polymer with the trade name Kevlar®. This polymer has a tensile strength-to-weight ratio ten times that of aluminum and six times that of drawn steel! The current efforts directed toward an all-plastic automobile show the high expectations for polymers and their capacity to reduce weight, save fuel, eliminate corrosion, and lower costs. This success is in no small part due to the chemist's ability to relate a polymer's mechanical properties to primary molecular data and fundamental principles of chemical bonding and conformational structure.

Another area of polymer research destined to lead to entirely new types of materials is connected with block polymers. These substances are deliberately designed so that they will "self-organize" into a continuous medium in which are lodged "microdomains." These "microdomains," regularly spaced through the solid, might be spheres, rods, or layers. They give new dimensions of control over the physical, optical, electrical, and magnetic properties of such solids. New devices, new applications, and new industries can be expected as chemists learn to control the intermolecular forces that account for the behavior.

The discovery of electrical conductivity in amorphous materials, in inorganic crystalline materials, and in organic polymers heralds a new era in the solid state field. It began almost fifteen years ago with the discovery that two-component organic crystals involving charge-transfer complexes could display metallic conductivity (the famous TTF-TCNQ). Now chemists have entered the field, bringing their talent for tailoring the structures to enhance desired properties. We are seeing large flat molecules (metallo-macrocycles) laced together with a string of covalently bound oxygen atoms to hold the charge-transfer units in a predetermined and rigidly enforced geometry. The polyacetylenes provide another prototype for a family of organic conductors. Even more glamorous are the inorganic materials polysulfur nitride and lead molybdenum sulfide that not only conduct well, they lose all electrical resistance at sufficiently low temperature (i.e., they become superconducting).

This catalogue of new materials and the new incentives for chemical syntheses they awaken could become much longer than time permits. The use of crystal defects to control crystal growth led to development of 1000-speed color film. The design of anisotropic molecules with preplanned charge distribution lies behind liquid crystal behavior that opened new markets in display technology. Microelectronics fabrication techniques depend upon carefully designed organic photoresists that are suitably sensitive to electron beams, x-rays, and ultraviolet light. "Anisotropic etching" of silicon chips is itself a challenging problem of chemistry at a gas-solid interface. Materials designed for extreme conditions answer needs in many modern technologies, including jet engines, automobile engines, nuclear and fusion reactors, and space craft heat shields. Perhaps the most awesome challenge to the chemist is to synthesize the next, next-generation of computer memory chips based upon molecular structures for information storage.

These exciting prospects are attracting more and more chemists to the materials sciences, a trend that DoE should encourage. The chemists' talents are not the only ones needed, but they are among the essential ones.

A PROGRAM PROPOSAL

It seems clear that the present state of excitement and opportunity in chemistry can and should be exploited to advantage by DoE in pursuit of its energy-oriented mission. This observation should perhaps remain in mind as the various DoE National Laboratories respond to the first recommendation in the May, 1983 Packard Report:***

"Recommendation 1.1 As a top management priority, Federal agencies should reexamine the missions of their laboratories."

As the missions of the DoE laboratories are redefined to bring them closer to the energy-related challenges currently faced by this nation, the likelihood is that chemistry must play a larger role.

In any event, the DoE chemistry programs are good and furnish a desirable starting point. The Briefing Panel examined carefully and in detail the current federal support level for fundamental research in the chemical sciences. It went on to estimate the investment needed to take advantage of the exciting prospects ahead. We became convinced that the priority areas A and B together warranted an immediate infusion of $50 million real growth into the NSF and DoE programs in chemistry. According to my reading of the President's budget, the DoE Energy Sciences Program proposes an FY 1985 combined operations and capital equipment budget of $89.7M ($80.9+8.8M). This provides a net increase of $7.7M for a 9.4% rise. This amount should be increased by $10M to $99.7M with the increment divided between operations and equipment to favor equipment. The DoE Materials Science Program, combining operations and capital equipment, has a proposed FY 1985 budget of $157.0M ($141.5+$15.5M). This is a net increase over FY 1984 by$19.1M, a 13.9% rise. This amount should be increased by $5M to $162.0M. Both of these added increments should be focussed on stimulation and support of the priority research areas A, Understanding Chemical Reactivity and B, Catalysis, as described in the Briefing Report on Selected Opportunities in Chemistry.

I thank you for letting me tell you about the Briefing Report and its relevance to the DoE programs you are considering today. I would be pleased to answer any questions about the Survey or about the testimony I have presented here today.

*** Report of the White House Science Council; Federal Laboratory Review Panel, May, 1983.

RESEARCH BRIEFINGS 1983

Report of the Research Briefing Panel on Selected Opportunities in Chemistry

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Research Briefing Panel on Selected Opportunities in Chemistry

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George C. Pimentel, Chairman
Research Briefing Panel on
Selected Opportunities in Chemistry

Preface

In 1982, on an experimental basis, the National Academies of Sciences and Engineering and the Institute of Medicine, through their joint Committee on Science, Engineering, and Public Policy (COSEPUP), developed research briefings on seven fields of science for the White House Office of Science and Technology Policy (OSTP), the National Science Foundation (NSF), and other interested federal departments and agencies. The seven fields were Mathematics, Atmospheric Sciences, Astronomy and Astrophysics, Agricultural Research, Neuroscience, Human Health Effects of Hazardous Chemical Exposures, and Materials Science. Each briefing, developed by a panel of experts, identified research areas within the field that were likely to return the highest scientific dividends as a result of incremental federal investment in fiscal year 1984. Briefing papers were prepared by each panel and published by the National Academy Press in early 1983.

Shortly thereafter, OSTP and NSF requested a second round of research briefings focused on federal investment opportunities in the fiscal year 1985 budget. COSEPUP agreed to this request and with the assistance of units of the National Research Council and through consultations with OSTP and NSF selected five new research briefing topics. These were as follows:

1. *Selected Opportunities in Chemistry*: Research directed toward enhanced understanding and application of three promising areas of chemistry: understanding chemical reactivity, chemical catalysis, and chemistry of life processes.
2. *Cognitive Science and Artificial Intelligence*: Research directed toward understanding how intelligent systems, animate or inanimate, deal with problems of communication, the acquisition of knowledge, and adaptive behavior.
3. *Immunology*: Research directed toward understanding the molecular, cellular, and intracellular processes of the immune system with a view to understanding control of the immune response and functions of the system.
4. *Solid Earth Sciences*: Research directed toward obtaining a new level of understanding of the structure, composition, energetics, and evolutionary history of the earth, with emphasis on the continental lithosphere and its margins.
5. *Computers in Design and Manufacturing*: Research directed toward understanding and enhancing the application of computers to product design and manufacture.

This document contains the report developed on one of these topics.

The second round of briefings was patterned after the first. Each one-hour briefing was developed by a panel of about 12 experts who met once for several days to assess the field and identify areas of unusual scientific opportunity. At each panel meeting a rapporteur was present to summarize the discussions and prepare an initial draft of a briefing paper. After further review by the panels, the briefing papers served as the bases of one-hour oral briefings presented to COSEPUP for review in early August 1983. Based on this review, the briefing papers were revised and served as the bases for oral briefings presented to federal officials in September and October 1983. Separate briefings were provided to Dr. George Keyworth, Science Advisor to the President, and selected members of his staff; Dr. Edward Knapp, Director of the National Science Foundation and senior members of the NSF staff; and senior representatives of other interested federal departments and agencies.

Funds to support both rounds of briefings were provided by the National Science Foundation.

George M. Low, *Chairman*
Committee on Science,
Engineering, and Public Policy

Report of the Research Briefing Panel on Selected Opportunities in Chemistry

EXECUTIVE SUMMARY

This is a time of special opportunity for intellectual advance in chemistry. It derives from our developing ability to probe and understand the elemental steps of chemical change and, at the same time, to deal with extreme molecular complexity. Powerful instrumental techniques are the crucial dimension. They account for the recent acceleration of progress that gives chemistry unusual promise for high return from additional resources.

Chemistry is a central science that provides fundamental understanding needed to deal with most societal needs: to feed the world population, to tap new sources of energy, to clothe and house humankind, to provide renewable substitutes for dwindling or scarce materials, to improve health and conquer disease, to add to our national security, and to monitor and protect our environment. Further, there can be no doubt that chemistry, with its current $12 billion positive balance of trade, is a crucial element in this nation's economic well-being. Our future international competitiveness will depend upon maintaining our present leadership position in the chemical sciences.

Directions of particular promise are becoming apparent in the course of the NAS/NRC study by the Committee to Survey the Chemical Sciences. This Committee is formulating a multi-year program to exploit the richest potentialities in a priority sequence that will maximize return on the needed additional federal investment. We identify here three areas, those that will yield the greatest rewards and furnish the appropriate beginning to this program.

A. Understanding Chemical Reactivity
B. Chemical Catalysis
C. Chemistry of Life Processes

A. *Understanding Chemical Reactivity*

We propose an initiative to apply the full power of modern instrumental techniques and of chemical theory to the clarification of factors that control the rates of reaction and to the development of new pathways for chemical change.

- *Molecular Dynamics*: to elucidate the entire course of chemical reactions, including the unstable atomic arrangements intervening between reactants and products.

- *Reaction Pathways*: to accelerate our rate of discovery of new reaction paths and new classes of compounds.

A principal objective of this initiative will be to provide the fundamental basis for U.S. leadership in development of new processes, new substances, and new materials.

B. *Chemical Catalysis*

We propose an initiative to apply the techniques of chemistry to obtain a molecular-level understanding of catalysts. Ultimately, new catalyst systems will result that will lay the foundation for the development of new chemical technologies. The program will emphasize research in four areas:

- *Heterogeneous Catalysis*: to apply the powerful new instrumental techniques of surface science to the study of chemistry on the surface of a solid.
- *Homogeneous Catalysis*: to take advantage of recent developments in synthetic chemistry that show promise as new soluble catalysts.
- *Photocatalysis and Electrocatalysis*: to investigate solution chemistry catalytically assisted by electrode processes, with and without absorption of light.
- *Artificial-Enzyme Catalysis*: to couple the chemists' ability to control molecular topography with the biochemists' understandings of natural catalysts so as to generate a new class of artificial enzyme-like catalysts tailored to specific needs.

A principal objective of this initiative will be to provide the fundamental knowledge and creative manpower required for the U.S. to maintain competitive advantage in catalysis-aided technologies.

C. *Chemistry of Life Processes*

We propose an initiative to develop and apply the techniques of chemistry to the solution of molecular-level problems in life processes. Research at this border between chemistry and biology requires individuals broadly competent in both areas, and a special effort must be made to develop such individuals. The program will emphasize the molecular aspects of six areas:

- Enzymology (understanding the molecular interactions responsible for enzymatic activity; production of natural enzymes for use as catalysts in chemical synthesis).
- Immunochemistry (the chemical basis of the immune and allergenic response; use, function, and modification of monoclone antibodies; synthesis of antigens and adjuvants).
- Chemical Endocrinology (synthesis of hormones and hormone analogs, especially those related to polypeptides).
- Neurochemistry (molecular basis of nerve transmission; neurotransmitters; agonist and antagonist chemistry; membrane polarization).
- Membrane Chemistry and Vectorial Chemistry (bioenergetics; active and passive transport).
- Biological Model Studies (host/guest chemistry; semisynthetic enzymes; properties of aqueous solutions; active site modeling).

A principal objective of this initiative will be to accelerate the conversion of qualitative biological information into techniques and substances useful in biotechnologies, in human and animal medicine, and in agriculture.

In the next two decades there will be dramatic changes in our basic understandings of chemical change and our ability to marshal those understandings to deliberate purpose. The program presented here is intended to define a leadership role for the U.S., as these advances are won. The rewards accompanying such leadership are commensurate with the prominent role of chemistry in addressing societal needs, in ameliorating the problems of our technological age, and in sustaining our economic well-being. The costs of falling behind are simply intolerable.

The need for enhanced federal investment in chemical research is rooted in a pattern of funding historically appropriate to a test-tube and bunsen burner era, an era long since eclipsed. The sophistication of a modern chemistry laboratory requires a much more vigorous financial commitment, both in capital investment and in supporting services. Even so, the cost is miniscule compared to the stakes involved; we must nurture a $175 billion industry that maintains a $12 billion positive balance of trade. We must provide it with a full reservoir of fundamental knowledge and we must attract a substantial share of our brightest young scientists to this rewarding task. This program can accomplish these goals.

Report of the Research Briefing Panel on Selected Opportunities in Chemistry

I. INTRODUCTION

This is a time of special opportunity for intellectual advance in chemistry. It derives from our developing ability to probe the elemental steps of chemical change and, at the same time, to deal with extreme molecular complexity. Powerful new instrumental techniques are the crucial dimension. They account for the recent acceleration of progress that gives chemistry unusual promise for high return from additional resources.

Chemistry is a central science that provides fundamental understanding needed to deal with most societal needs. It is a critical component in Man's attempt to feed the world population, to tap new sources of energy, to clothe and house humankind, to provide renewable substitutes for dwindling or scarce materials, to improve health and conquer disease, to add to our national security, and to monitor and protect our environment. Basic research in chemistry will surely help future generations cope with their evolving needs and unanticipated problems.

Chemistry is also a crucial element in this nation's economic well-being. The U.S. Chemical and Allied Products industry employs over a million people, makes manufacturing shipments totaling about $175 billion, and currently displays a $12 billion positive international balance of trade, second highest of all commodity groups. Our competitiveness in a range of international markets depends upon maintaining our present position of leadership in the chemical sciences. There is no area of basic science that offers a more secure investment in the Nation's future.

Thus, rapid advances are possible now in chemistry, advances that will continue to enrich our cultural heritage, that will ultimately respond to human needs, and that will sustain our economic competitiveness. Directions of particular promise have become apparent in the course of the NAS/NRC study by the Committee to Survey the Chemical Sciences. This Committee is formulating a multi-year program to exploit the potentialities in a priority sequence that will maximize return on the needed additional federal investment. We identify here three areas that furnish the appropriate beginning to this program.

A. Understanding Chemical Reactivity
B. Chemical Catalysis
C. Chemistry of Life Processes

II. PRIORITY OPPORTUNITIES

Three priority thrusts are described. The first is connected with opportunities to understand, in the most fundamental sense, chemical reactivity and to control it. The second is to advance our understanding of catalysis in all of its facets. The third will extend to the molecular level our understanding of life processes. These three thrusts are complementary and reinforcing in the sequence given. They have different rationales and distinct budget needs, so they are presented separately.

A. *Understanding Chemical Reactivity*

1. *Program.*

We propose an initiative to apply the full power of modern instrumental techniques (lasers, molecular beams, computers, etc.) and of chemical theory to the clarification of factors that control the course of a chemical reaction and to the development of new pathways for chemical change.

- *Molecular Dynamics*: to elucidate the entire course of chemical reactions, including the unstable atomic arrangements intervening between reactants and products.
- *Reaction Pathways*: to accelerate our rate of discovery of new reaction paths and new classes of compounds.

2. *Objectives.*

- To advance our fundamental understanding of chemical reactivity.
- To attract exceptional young scientists to the frontiers of this understanding.
- To apply this understanding to the development of new types of reaction and new classes of compounds.
- To provide the fundamental basis for U.S. leadership in development of new processes, new substances, and new materials.

3. *Rationale.*

Public support for basic research is justified, in part, on cultural grounds and, in part, on practical grounds. Our culture includes the premise that learning about ourselves and our environment is an ample basis for encouragement of scientific investigations. In addition, we recognize that our increasing ability to meet the common desire for survival, comfort, health, and freedom from toil is rooted in our increasing comprehension of what goes on within and around us.

Within the cultural basis for science, three prime questions stand out: the structure of the Universe, the makeup of matter, and the mechanism of life processes. The third is probably the strongest human preoccupation: the nature and preservation of life. Since all life processes—birth, growth, reproduction, aging mutation, death—are manifestations of chemical change, understanding chemical reactivity can be seen as the foundation for our ultimate understanding of life. Thus chemistry, along with biology, can properly be placed with astronomy and high energy physics as scientific investigations justifiable because they contribute to human knowledge in areas of universal philosophical significance.

However, that does not complete the justification for increasing our understanding of chemical reactivity. It is just as convincingly based upon practical grounds. The development of new processes and new materials depends upon our understanding and control of chemical change. Fundamental advances here will present avenues for innovation that can be exploited in the study of combustion, corrosion and electrochemistry, polymer formation, tailored organic molecules, and new solid state materials. It responds to our need to develop new energy sources, to provide alternate materials for nonrenewable or scarce materials, and to maintain economic competitiveness, all while attentively protecting our environment. It permits the U.S. to produce billions of pounds of organic chemicals, at low cost, in high yield, and with minimum waste product. Combined with our 1981 production of 9.8 billion pounds of synthetic fibers (such as polyesters), 28 billion pounds of plastics (such as polyethylene) and 4.4 billion pounds of synthetic rubber, this capability accounts for the total business volume mentioned earlier, an amount exceeding $175 billion with its current international trade surplus of $12 billion.

This is surely a time of special opportunity to deepen our fundamental knowledge of why and how chemical changes take place. The advance of the frontiers of molecular dynamics has undergone a revolutionary acceleration during the last decade. At the same time, synthetic chemists are exponentially increasing the number of known molecular structures, and constantly adding to our arsenal of reaction types and classes of compounds. Much of this can be attributed to the development and application, during the last two decades, of an array of powerful instrumental and analytical techniques. A few examples show that we have new capabilities in hand with which to probe far beyond current frontiers.

MOLECULAR DYNAMICS

Lasers by themselves have spectacularly expanded our experimental horizons over the last decade. Their short pulse durations permit easy probing of chemical reactions that occur in less than a millionth of a second down to times a thousand-fold shorter (from a microsecond to a nanosecond). With more complex (and more expensive) equipment, chemists are now entering a time domain still another thousand-fold shorter (to a picosecond). Lasers also provide tunable, extremely narrow frequency light sources, implying vastly greater diagnostic sensitivity and selectivity. Finally, lasers give us extremely high light intensities, either in the form of short pulses of ultrahigh power or as continuous light sources with unprecedented photon flux.

Computers also make important contributions to this revolution, both in experimental and theoretical chemistry. They are now common components of experimental assemblies and a number of the chemist's more sophisticated instruments have built-in (dedicated) computer capability as an essential element. (For example, fourier transform infrared spectrometers, fourier transform nuclear magnetic resonance spectrometers, and X-ray spectrometers). Furthermore, today's computing capability has brought *ab initio* calculations and chemical theory to new levels of fruition.

These are only exemplars—a host of sophisticated instrumental methods ought to be mentioned: molecular beams, ion cyclotron resonance, electron spin resonance, photoelectron spectroscopy, magnetic circular dichroism, resonance Raman, Mossbauer, etc. All of these account for the rich possibilities lying before us. However, the historical basis for funding basic research in chemistry was not premised on the existence (and cost) of such sophisticated equipment. One of the strongest arguments for a large increase in federal support for chemical research is that existing levels do not provide sufficient access to these state-of-the-art techniques and without them, U.S. science will fall behind in areas crucial to our national well-being.

Turning to these new frontiers, the advance of understanding of *molecular dynamics* is one of the most rapidly moving. Here are some of the new phenomena we can now explore.

- *Fast chemical processes in real time.* The primary processes of numerous chemical changes are determined by dynamical events that are intrinsically fast. Many solution phase reactions, photochemical reactions, electron solvation, molecular reorientation in liquids, and reactions of certain biological systems can now be watched "in real time" on the nanosecond-to-picosecond time scale.
- *Energy transfer and movement.* In all chemical changes, the pathways for energy movement are determining factors. Competition among these pathways (including energy dissipation) determines the product yields, the product-state distributions, and the rate at which reaction proceeds. Chemists are

now able to track these pathways: radiation, internal conversion, intersystem crossing, intramolecular and intermolecular energy transfer, unimolecular decomposition.

- *Ab initio calculations of reaction surfaces.* With today's computers, the structure and stability of any molecular compound with up to 3 first-row atoms (carbon, nitrogen, oxygen, fluorine) plus various numbers of hydrogen atoms can be calculated almost to the best accuracy available through experiment. This opens to the chemist many situations not readily accessible to experimental measurement. Short-lived reaction intermediates, excited states, and even saddle points of reaction can now be understood, at least for small polyatomic molecules. In a major advance, we can now calculate the forces on all of the atoms during their reorganization from reactant to product molecule geometries.
- *State-to-state chemistry.* Major developments in molecular beam technology, including mass spectrometric ("universal") detectors, vacuum technology, laser excitation, and supersonic jet sources, have enormously broadened their applicability. In the ultimate experiment, reactants can be brought together in precisely known energetic states, with every quantum number fixed, and then the product energies and relative probabilities can be established in the same detail.
- *Mode-selective chemistry.* With high-power, sharply tunable lasers, it is possible to excite one particular degree of freedom for many molecules in a bulk sample. As long as this situation persists, such molecules react as if this degree of freedom is at a very high temperature while all the rest of the molecular degrees of freedom are cold. The chemistry of such selective excitation could potentially reveal the importance and role of that particular degree of freedom in facilitating reaction. To extract this valuable information, energy redistribution and relaxation must be brought under control, and this frontier is being explored.
- *Multiphoton excitation.* One of the most surprising discoveries of the 1970's was that powerful pulsed lasers could highly excite the vibrational degrees of freedom of a molecule on a time scale short compared to molecular collision times. With many tens of quanta of vibrational excitation, the molecule displays unusual chemical pathways. This opens a new type of photochemistry with unique possibilities, the first of which to be recognized was isotope enrichment.

The rich potentialities of these techniques promise to show us how reactions proceed over their entire course. We will at last be able to understand the unstable situations intervening between reactants and products. To realize these benefits, there must be wider access to the sophisticated instrumentation (including computing capability) and the cadre of bright young scientists attracted to this area must be encouraged and increased.

REACTION PATHWAYS

A manifestation of this increasing understanding and control of chemical reactivity is the rapid advance now taking place in devising new reaction pathways in synthetic chemistry. This progress presents a high leverage opportunity since herein lies the foundation of future developments of new products and new processes.

Again powerful instrumental techniques play a central role. The rapid and definitive identification of reaction products, both in composition and structure, accounts for the speed with which synthetic chemists are able to test and develop their synthetic strategies. The nuclear magnetic resonance and mass spectra show what elements are present and the structural environment of virtually every atom. The X-ray crystal structure reveals the complete molecular structure: the interatomic distances, bond angles, and even the right- or left-handedness when mirror-image relationships are present. Spectroscopic techniques, as well, have been essential to progress in the rapidly developing area of organometallic chemistry. The visible and infrared spectra of transition metal complexes reveal electronic configurations and bonding, the foundation for clarifying mechanisms for ligand substitution and electron-transfer processes.

- *Selective pathways in organic synthesis.* Selectivity is the key challenge to the synthetic chemist—to make a precise structural change to a single desired product. The different intrinsic reactivity in each bond type must be recognized (chemoselectivity), reactants must be brought together in proper orientation (regioselectivity) and the desired three-dimensional spatial relations must be obtained (stereoselectivity). The degree to which this type of control can be achieved is shown in the synthesis of the substance adamantane ($C_{10}H_{14}$). This novel molecule resembles in structure a 10-atom "chip" off of a diamond crystal. In a *tour de force,* it was originally produced by a many-step process in only 2.4% yield. Recent research in polycyclic hydrocarbon synthesis now gives adamantane in one step in 75% yield. Then, a surprise practical payoff came when it was discovered that adding a single amine substituent to adamantane gave adamantine (1-amino-adamantane), which proved to be an antiviral agent, a prophylactic drug for influenza, and a drug to combat Parkinson's disease.

The recent development of new ways to construct cyclic five-membered rings has again paid off handsomely. The diverse array of applications includes production of thienamycin, $C_{13}H_{14}N_2SO_4$, a novel relative of penicillin and an important new drug. At another extreme, large ring compounds have been exceptionally difficult to synthesize. Their structures are complicated by functionally crucial left/right-handed structural geometrics ("chiral centers"). Their wide ranging biological properties—from pleasant fragrances for perfumes to anti-fungal, antitumor, and antibiotic activities—make large ring synthesis an interesting challenge. An example is erythromycin, $C_{37}H_{68}O_{12}N$, which in the desired atomic hookup can be shaped into 262,144 different structures derived from the many possible ways to couple the right- and left-handedness at its 18 chiral centers ($2^{18} = 262,144$). Twenty-five years ago, this compound was judged to be "hopelessly complex" by R. B. Woodward, who won the Nobel Prize for synthesizing molecules as complex as quinine and vitamin B_{12}. Today we can aspire to such a goal, in part because of the development of specially designed templates that bring together the terminal atoms of a fourteen-atom chain to form a fourteen-membered ring. This provides the structural framework of erythromycin and it has already resulted in the synthesis of a number of constituents of musk and contributed to our understanding of smell.

- *Crossing inorganic/organic boundaries.* The traditional line of demarkation between organic and inorganic chemists has virtually disappeared as the list of fascinating metal-organic compounds continues to grow. The ubiquitous appearance of these compounds in biological systems underscores the importance of encouraging this cross-boundary research. Furthermore, research in developing new inorganic substances has provided a surprising dividend in their frequent applicability in organic synthesis.

The latter situation is illustrated by the borohydrides. The cohesive picture we have, at last, for this strange boron/hydrogen family was not possible before their study by X-ray crystallography, infrared and NMR spectroscopy, and molecular orbital theory. Now borohydrides are widely used as selective, mild reducing agents in organic synthesis. Silicon and transition-metal organometallic compounds give other examples. Silicon compounds, for example, are used to fold an extended molecular reactant precisely as needed to synthesize the molecule cortisone. Now this valuable therapeutic agent can be made in less than 20 steps at a yield 1000 times higher than achieved in the earlier 50-step process.

Compounds with metal atoms sandwiched between organic rings continue to proliferate and their chemistry will likely relate to catalysis. The metal-organic complexes provide another active synthetic field, with interest both in catalysis and, perhaps, in radioactive or metal-waste cleanup.

- *Novel solids*. Chemists are learning how to prepare solids with quite remarkable properties. Thus, families of solid substances are being synthesized which, like the alumina-silicates (the "zeolites"), are deliberately contrived to include particular shaped cavities and channels. Guest molecules that slip comfortably into these channels can be held in favored conformations as reactants bring about desired chemical changes. The result is that only particular molecules (the ones that fit) react and they do so in a structurally specific way. Entirely different sorts of solids are giving new families of electrically conducting materials. The lead molybdenum sulfide, $PbMo_6S_8$, is a superconductor that can remain superconducting up to 600 kilogauss fields. One of the several conducting organic materials is polyacetylene which, on exposure to various chemicals (iodine, arsenic trifluoride, etc.), can approach metallic conductivities. Polysulfurnitride, $(SN)_x$, not only rivals metal conductivity, it also displays superconductivity. Another promising class of new linear-chain polymer conductors are those based upon metallo-macrocycle complexes held together by bridging groups and treated with an electron-accepting compound. This class is amenable to a wide range of electronically significant chemical modification, hence tailoring to intended application.

Pressure as a controlling dimension of solid state reactions has long been recognized but little understood. With techniques now available, solids can be compressed and studied spectroscopically up to a few hundred thousand atmospheres pressure. New molecular structures, reactivities and electronic properties can be obtained. Photochromic materials provide an example. Substances like the anils, spiropyranes, and bianthrones change color when exposed to light. Under pressure, the colors can be "tuned" and some of these materials will display the color change merely by heating, without the need for exposure to light. These effects are attributable to changes in molecular structures and electronic makeup which, in turn, can affect chemical reactivity.

Solid state chemistry is relatively less active in the U.S. than abroad; French, German, and Japanese chemists have leadership positions. Hence, there can be a high return if more activity can be stimulated here in the synthesis and characterization of radically new solids. There will emerge new semiconductors, solid state ionic materials (used in batteries, memory devices, display devices, and chemical sensors), ferroelectrics, pyroelectrics, and magnetic materials. Creative synthetic chemists must be attracted and encouraged in this area.

- *Pathways using light as a reagent*. Another promising chemical pathway is connected with the use of light photons in chemical synthesis. Many organic molecules display quite different chemistry and structures after absorption of light. Photosynthesis provides the most striking prototype and our understanding is advancing rapidly. "Artificial photosynthesis" both mimicking Nature and generalizing into new directions is under active study. Chemical storage of solar energy is an obvious long-term goal. In addition, new routes in chemical synthesis are offered. Some high energy ("strained") molecular structures, including those of many natural products, must be formed in energy-consuming (endothermic) processes (e.g., the mycin antibiotics, certain alkaloids, vitamin D precursors, and certain steroid hormones). It is difficult to put in this energy because the active reagents tend to threaten the fragile product. In the photochemically induced process, less aggressive reactants can be used which can be excited with light to approach the product gently from above, with delicate control through the photolysis wavelength. A single example shows the great potential. A calcium homeostatic steroid hormone with the formula $C_{26}H_{44}O_2$ (1,25-dihydrovitamin D_3) can be synthesized photochemically. By using tuned laser light controlled to the optimum wavelength (300nm), the synthetic yield of the desired structure has been increased 400%. How important such light-assisted chemistry will be remains to be seen. Chemists understand the ground state (unexcited) chemistry of literally millions of compounds. Virtually every one of these compounds has different chemistry after light absorption but we have explored only a miniscule fraction of this new domain!

4. *Collaboration*

The thrust toward *understanding chemical reactivity* has inviting avenues for collaboration across traditional disciplinary boundaries. Much of the most fundmental work on molecular dynamics is at the chemistry-physics interface and it specially benefits from close interaction between chemists and physicists on the one hand and between experimentalists and theoreticians on the other. In a similar way, exciting new horizons in synthesis are bringing together the perspectives and techniques of individuals who used to be differentiated as inorganic or organic chemists. Collaborative mechanisms should be encouraged.

B. *Chemical Catalysis*

1. *Program.*

We propose an initiative to apply the techniques of chemistry to obtain a molecular-level understanding of catalysts. Ultimately, new catalyst systems will result that will lay the foundation for the development of new chemical technologies. The program will emphasize research in four areas:

Heterogeneous catalysis: to apply the powerful new instrumental techniques of surface science to the study of chemistry on the surface of a solid.

- *Homogeneous catalysis*: to take advantage of recent developments in synthetic chemistry that show promise as new soluble catalysts.
- *Photocatalysis and electrocatalysis*: to investigate the rich possibilities of solution chemistry catalytically assisted by electrode processes, with and without absorption of light.
- *Artificial-enzyme catalysis*: to bring together chemists' ability to synthesize molecules of predesigned topography and the biochemists' emerging understandings of natural catalysts, the enzymes. We should be able to generate a new class of artificial enzyme-like catalysts tailored to specific needs.

2. *Objectives.*

- To identify the fundamental molecular ingredients of catalytic processes in order, ultimately, to guide the development of chemical high technology.
- To synthesize new catalysts that may serve as the foundation of new chemical processes.
- To increase the number of young scientists who have the breadth and background needed to contribute to the field of chemical catalysis.
- To provide the fundamental knowledge and creative manpower required for the U.S. to maintain competitive advantage in catalysis-aided technologies.

3. *Rationale.*

A catalyst accelerates chemical reactions toward equilibrium without being consumed. This acceleration can be as much as ten orders of magnitude. A *selective* catalyst can have this same dramatic effect but on only one of many competing reactions. While the development of new catalysts was empirical fifteen years ago, research innovations in chemical sciences over the last ten years are converting catalysis from art to science. A familiar example displays the benefits to be gained—the catalytic converter developed for automobiles to reduce air pollution. The catalyst—containing two grams of platinum, palladium, and rhodium per car—oxidizes unburned hydrocarbons and carbon monoxide to harmless water and carbon dioxide. Simultaneously, it reduces toxic nitrogen oxides to harmless nitrogen gas.

Estimates that twenty percent of the gross national product is generated through the use of catalysis demonstrate the major role industrial catalysis has in satisfying such diverse societal needs as food production, energy conversion, defense technologies, environmental protection and health care. On the horizon is the extensive use of catalysts to tap new energy sources—such as heavy oils, coal, oil shale, tar sands, lignites, and biomass—as we run out of oil. However, American preeminence in catalysis science is now challenged by Japan, Germany, the USSR, and France. These countries have established institutional networks to accelerate research and development in this evolving high-technology field. To meet this challenge, we must keep our own catalytic science vital.

Industrial research in catalysis is critically dependent on the techniques and concepts which have been developed in university and National Laboratories. Since industrial laboratories use the latest surface science and laser spectroscopic techniques, they want their new young scientists to bring with them state-of-the-art experience. Furthermore, industrial catalysis research must be chosen with an eye toward existing technology and product lines. Industry cannot sustain the adventurous fundamental research that will underlie the discovery of radically new catalysts. To illustrate this, consider the enormously important conversion of atmospheric nitrogen into ammonia. The original work by Haber in Germany produced an ammonia yield of 13% per pass. Today the same process is used on a massive scale. Yet, seventy years after Haber's work, a modern ammonia unit producing some 1500 tons per day operates at only slightly greater yield per pass (perhaps 15%). There is no physical limitation here—equilibrium is on our side. What is needed is fundamental research in catalysis. This is a role for university chemists. It is a place for federal investment.

This chemical catalysis program will concentrate on long-term research to learn about catalytic processes on the molecular level. Then the new fundamental knowledge generated will be transferred into technology by the employment of the emerging young scientists in industry and by the ties formed in this program among scientists in the universities, the National Laboratories and industry.

HETEROGENEOUS CATALYSIS

Heterogeneous catalysts are solid materials prepared with large surface areas (1-500 m^2/g) upon which chemical reactions occur at extremely high rate and selectivity. Some major new commercial processes based on heterogeneous catalyst developments in recent years include:

—"reforming" hydrocarbons to high octane composition (platinum alloy catalysts);
—"cracking" high paraffins to gasoline (molecular sieve catalysts);
—methanol to gasoline, jet fuel (molecular sieve catalysts);
—exhaust converter on automobiles (platinum, palladium, rhodium catalysts);
—ethylene oxidation to ethylene oxide (silver, cesium, chlorine catalyst);
—propylene oxidation to acrolein and acrylonitrile (bismuth, and molybdenum oxide catalyst);
—ethylene polymerization (chromium catalyst);
—propylene polymerization (titanium, magnesium oxide catalyst).

Surface science is developing rapidly and now gives us experimental access to this two-dimensional reaction domain. Because of the unsatisfied bonding capability of the atoms at the surface, chemistry here is dramatically different from that of the same reactants brought together in solution or the gas phase. But when chemists are able to "see" what molecular structures are on the surface, then all of our knowledge of reactions in conventional settings becomes applicable. This will open the door to understanding and controlling the chemistry in this surface domain. There are five areas of heterogeneous catalysis where this understanding will have major impact on new chemical technologies.

- *Molecular sieve synthesis and catalysis.* Molecular sieves are crystalline alumina-silicates containing pores or channels within which chemical reactions can be initiated. They offer unparalleled efficiency both for cracking of petroleum and for conversions such as shale oil or methanol to gasoline. We need to know better how to synthesize molecular sieves with controlled molecular pore size, as well as to determine the elementary reaction steps and intermediates that account for their efficacy.
- *Metal catalysis.* Finely dispersed transition metals are already coming into use to catalyze hydrocarbon conversions and ammonia synthesis for fertilizers. Other such applications and improved performance will follow from intensive research into the control of surface structures, oxidation states, residence time of reaction intermediates, and resistance to catalyst "poisons" (such as sulfur).
- *Substitutes for precious metal catalysts.* Many of the most effective catalysts are rare metals not available in the U.S., including rhodium, platinum, palladium, and ruthenium. Their strategic value requires a concerted research effort to find more accessible substitutes, such as transition metal oxides, carbides, sulfides, and nitrides.
- *Conversion catalysts.* We must find catalysts to convert abundant substances to useful fuels and industrial feedstocks. These reactions include conversion of atmospheric nitrogen to nitrates, methane to methanol, carbon dioxide to formate, and depolymerization of coal and biomass to useful hydrocarbons.
- *Catalysts to improve air and water quality.* We have many environmental pollution problems for which we need to match the spectacular success of the catalytic converter used to clean automobile exhaust gases. To begin, we need catalysts that remove sulfur oxides from smoke plumes, that purify water, and that prevent acid rain.

As we learn more about the molecular structures at the solid-gas interface (reactants, intermediates and products), a better understanding of surface chemical bonding will follow. We can look forward to understanding additives that modify catalyst performance ("promoters" and "poisons"). Then, the challenging subject of synthesis of the designed catalyst can be addressed. All of this fundamental knowledge will underlie and facilitate the development of new and more selective heterogeneous catalysts.

HOMOGENEOUS CATALYSIS

Homogeneous catalysts are soluble and active in a liquid reaction medium. Often they are complex metal-containing molecules whose structures can be modified to tune reactivity in desired directions to achieve very high selectivities. (In this sense homogeneous catalysts can be superior to heterogeneous ones.) The largest industrial-scale process using homogeneous catalysis is the partial oxidation of para-xylene to terephthalic acid (United States production in 1981 was 6.2 billion pounds per year), which uses dissolved salts of cobalt and manganese as the catalyst system. Most of the product ends up polymerized to give us polyester clothing, tire cord, soft drink bottles, and a host of other useful articles.

An important branch of homogeneous catalysis has developed from research in organometallic chemistry. An example is rhodium dicarbonyl diiodide, employed in the commercial production of acetic acid from methanol and carbon monoxide. With this catalyst present, the reaction economically gives more than 99% selectivity to acetic acid.

There are three areas of homogeneous catalysis with potential for major impact on new chemical technologies from increased understanding.

- *Activation of inert molecules*. There are a number of relatively inert molecules that are enticing as reaction feedstocks because of their abundance: nitrogen, carbon monoxide, carbon dioxide, and methane. One way to approach this end might be through homogeneous organometallic catalysis. Dramatic examples of this promise are beginning to appear. Soluble compounds of tungsten and molybdenum with molecular nitrogen have been prepared and induced to produce ammonia under mild conditions. The carbon-hydrogen bonds in normally unreactive hydrocarbons have been split by organorhodium and organoiridium complexes. Hope for build-up of complex molecules from one-carbon molecules, such as carbon monoxide, is encouraged by recent demonstrations of carbon-carbon bond formation at metal centers bound in soluble metal-organic molecules. Synthesis of compounds with multiple bonds between carbon and metal atoms has had a major impact in clarifying the catalytic interconversion of olefins. While there is much to learn, the stakes are high and the odds for success are excellent.
- *Metal cluster chemistry*. An adventurous frontier of catalysis lies in the expanding capability of chemists to synthesize molecules built around several metal atoms in proximity (a "metal cluster"). In parallel, solution and cryogenic techniques are revealing the structures and chemistry of small aggregates containing only metal ions or atoms ("naked clusters"). All of these clusters, bound or "naked", furnish a natural bridge between homogeneous catalysis and bulk metal, heterogeneous catalysis.

  Many directions are being explored. Cubical units of four metal atoms and four sulfur atoms are now known for iron, nickel, tungsten, zinc, cobalt, manganese, and chromium. This "cubane" structure for iron has been found to be the functional unit in the ferrodoxin iron proteins that catalyze electron transfer reactions in biological systems. Many cluster compounds have been made from metals bound to carbon monoxide. These metal carbonyls have formulas $M_x(CO)_y$, and x can be made very large. (The world's record as of this writing is a platinum compound with $x = 38$.) It is intriguing that many of the most catalytically active metals also form cluster compounds (e.g., rhodium, platinum, osmium, ruthenium, iridium, etc.). Now the chemistry of these elements can be studied as a function of cluster size.
- *Stereoselective catalysts*. Another exciting frontier involves the development of homogeneous stereoselective catalysts. Many biological molecules can have either of two geometric structures connected by mirror-image (chiral) relationships, and generally only one of these structures is functionally useful in the biological system. If a complex molecule has seven such chiral carbon atoms and a synthetic process produces all of the mirror-image structures in equal amounts, there would be $2^7 = 128$ structures, 127 of which might have no activity or, worse, some undesired effect. Thus the ability to synthesize preferentially the desired structure with the desired geometry at every chiral center is essential.

  Immense strides in this area are being made. For example, L-dopa, an amino acid that has revolutionized the treatment of Parkinson's disease, is now made using an asymmetric addition of hydrogen to a carbon-carbon double bond. The catalyst is a soluble rhodium phosphine catalyst that gives 96% of the correct structure with high efficiency. Stereospecific oxidations can also be carried out. The recent invention of a titanium catalyst to add, in a specific geometry, an oxygen atom across a carbon-carbon double bond has lowered the price of gypsy moth attractant ten-fold. Despite these successes, the basic factors that produce stereochemical control are not at all well understood. Mechanistic studies are needed and the rewards from better understanding will be great.

Future advances in homogeneous catalysis are dependent upon easy access to advanced instrumental techniques: X-rays, high-field nuclear magnetic resonance, electron spin resonance, mass spectroscopy, and computational facilities. Further, work at the interfaces between organic, inorganic and physical chemistry is involved, so breadth of knowledge is especially important.

PHOTOCATALYSIS AND ELECTROCATALYSIS

Exciting advances have recently been made in the study and control of chemistry taking place at the interface between a liquid solution and an electrochemical electrode surface. In some applications, the chemistry is initiated by absorption of light by a semiconductor used as an electrode. Whether light is involved (photocatalysis) or not (electrocatalysis), this rapidly moving field depends upon our knowledge both of homogeneous catalysis and of semiconductor behavior.

- *Photoelectrochemical cells.* There is considerable promise from research directed toward conversion of light to electrical energy in a photoelectrochemical cell. In such a cell, one or both of the electrodes is a semiconductor material that absorbs the incident light. The lure is that semiconductors, probably with chemically modified surfaces, can absorb red and infrared light, the spectral region within which most solar energy falls.

Chemists are learning how to bond dyes and protective polymers to the surface of a semiconductor solid through covalent bonds. There is now the potential for solving the key problems of photoelectrochemical cells: to catalyze the essential electron-transfer reactions with solution species, to prevent chemical erosion of the electrode, to avoid back-reaction, and to shape the active spectral region to match that of the energy source, the sun. Already cells for conversion of solar energy to electrical energy have rivaled those of solid state photovoltaic cells (e.g., the n-GaAs/selenide system operates at 14% efficiency). Numerous "non-conventional" semiconductors are under investigation, such as TiO_2, CdS, WSe_2. These materials are still speciality products but there is good prospect that they will cost much less than existing single crystal photovoltaic materials.

- *Photocatalysis.* Related studies involving photoelectrochemical cells or suspensions of semiconductor materials focus attention on the chemistry that can be brought about. In these systems, light absorbed in the semiconductor promotes catalytic oxidation-reduction chemistry at the electrode-solution or at a membrane-solution interface. Such oxidation-reduction chemistry has significant scientific interest and, likely, great practical significance. For example, photodestruction of a toxic waste material such as cyanide has been demonstrated at titanium dioxide surfaces. A more popularized and perhaps feasible concept is that such photocatalytic chemistry, solar energy driven, could produce massive amounts of hydrogen and oxygen from the photoelectrolysis of water. What an intriguing prospect, to convert from diminishing and seriously polluting petroleum fuels to a renewable fuel that burns to water and that is made from water using energy from the sun.
- *Electrocatalysis.* Apart from light-initiated processes, electrode surfaces with catalytic activity offer a new domain for chemical synthesis. In a field with a long heritage, recent developments have shown that electrode surfaces can be chemically tailored to promote particular reactions. This research area

has adopted techniques from the semiconductor industry (such as chemical vapor deposition) and coupled them with imaginative synthetic chemical techniques for surface modification.

An example is the electrocatalyst family developed for use in chlorine generation in chlor-alkali cells. A successful case is based upon a thin layer of ruthenium dioxide (the catalyst) deposited on a base metal electrode. This electrocatalyst has dramatically changed practice in the chlor-alkali industry (an industry representing billions of dollars in sales) because of its improved energy efficiency and reduced cell maintenance. Future developments will include radically improved fuel cells, which provide clean and thermodynamically efficient conversion of chemical fuels to electricity.

- *Chemistry at the solid/liquid interface.* Before the technological potentialities of any of the above can be realized, we must have a much better understanding of the nature of chemistry at the semiconductor/liquid interface. The marvelous instrumentation developed for surface science studies is, of course, applicable only at solid/vacuum interfaces. We need comparable capability at the solid/liquid boundary. This capability will be won from fundamental research in solid state chemistry, electrochemistry, surface analysis, and surface spectroscopy. Where the biggest gains are to be made is a speculative question. The surprising discovery of the million-fold intensification involved in surface-enhanced Raman effect encourages optimism.

The potential gains from these exciting areas are considerable. We need to know how to catalyze multielectron transfer reactions at an electrode surface. That is the chemistry required, for example, to photogenerate a liquid fuel such as methanol from carbon dioxide and water. Multielectron transfer catalytic electrodes for oxygen reduction in electrochemical cells would find a welcoming home in the fuel cell industry.

It is also likely that research on semiconductor electrode surface modification will reflect back beneficially into the field of electronics. Thus, the integrated circuit technology based upon GaAs may depend upon control of its surface chemistry. Already photoresist/chemical etching techniques are recognizing the importance of the chemistry involved in surface modification (witness the pursuit of "anisotropic chemical etching").

In summary, our evolving understanding of the electrode/solution interface, buttressed by concepts based on semiconductor electrodes and the development of a number of new methods for modifying electrode surfaces, has provided powerful new approaches to both photocatalysis and electrocatalysis. Future advances will benefit synergistically from progress in heterogeneous and homogeneous catalysis, increased understanding of mass and charge transport within the electrode surface layers, and continued development of experimental methods and theoretical models for the interface.

ARTIFICIAL-ENZYME CATALYSIS

The most striking benefit from our bounteous knowledge of reaction pathways and the analytical capacity of modern instrumentation has been the development of capability to deal with molecular systems of extreme complexity. With the synthetic chemist's prowess and such diagnostic instruments as nuclear magnetic resonance, X-ray spectroscopy, and mass spectroscopy we can now synthesize and control the structure of molecules that approach biological complexity. This includes the ability to fix the molecular shape, even extending to the mirror-image properties that are so crucial to biological function.

There is no application of these capabilities more intriguing than coupling them with our growing knowledge of catalysis to synthesize artificial enzymes. In Nature, enzymes are the biological catalysts that accelerate a wide variety of chemical reactions at the modest temperatures at which living organisms can survive. A given enzyme selects from a many-component system a single reactant molecule and transforms it to a single product with prescribed chiral geometry.

Without catalysts, many simple reactions are extremely slow under ambient conditions. Raising the temperature speeds things up, but this may include a variety of undesired outcomes—acceleration of unwanted reactions, destruction of delicate products, and waste of energy. Hence, there are strong reasons to develop synthetic catalysts that work like enzymes. First, natural enzymes do not exist for most of the chemical reactions in which we have interest. In the manufacture of polymers, synthetic fibers, medicinal compounds, and many industrial chemicals, very few of the reactions used could be catalyzed by naturally occurring enzymes. Even where there are natural enzymes, their properties are not ideal for chemical manufacture. Enzymes are proteins, sensitive substances that are easily denatured and destroyed. In those industries that do use enzymes, major effort is directed toward modifying them to make them more stable.

- *Controlled molecular topography and designed catalysts.* We have a pretty good idea how enzymes work. Nature contrives a molecular surface fitted to a specific reactant. This surface attracts from a mixture the unique molecular type desired and immobilizes it. Held on the surface, the selected reactant is forced to abandon its flexibility and assume a distinct shape. When the reaction partner arrives, the scene is set for the desired reaction to take place in the desired geometry.

Organic chemists who have taken up this challenge are making excellent progress. Without special control, large molecules usually have exclusively convex surfaces (ball-like shapes). So a first step has been to learn to synthesize large molecules with concave surfaces. Then, these concave surfaces could be shaped to accommodate a desired reactant. Cyclodextrins provide examples—they are toroidal in shape. The crown ethers, developed over the last 15 years, have a quite different surface topography. For instance, 18-crown-6 consists of twelve carbon atoms and six oxygen atoms evenly spaced in a cyclic arrangement. In the presence of potassium ions, the ether takes up a crown-like structure in which the six oxygen atoms point toward and bind a potassium ion. Lithium and sodium ions are too small and rubidium ions too large to fit in the crown-shaped cavity, so this ether preferentially extracts potassium ions from a mixture. Much more ornate examples now exist. Chiral binaphthyl units can be coupled into cylindrical or egg-shaped cavities. With benzene rings, enforced cavities have been made with the shapes of bowls, pots, saucers, and vases.

Plainly we are moving toward the next step, to build into these shaped cavities a catalytic binding site. The earliest successes will likely be patterned after natural enzymes but there is no doubt that in time, artificial, enzyme-like catalysts will not be limited by what we can find already known in Nature.

- *Biomimetic enzymes.* A short-cut approach is to pattern artificial enzymes closely after natural enzymes. This has been called "biomimetic chemistry." As examples, mimics have been prepared for the enzymes that biologically synthesize amino acids. The artificial enzymes incorporate the important catalytic groups of a natural enzyme (vitamin B_6, for example) and show good selectivity, even including the formation of the correct chirality in the product. Mimics have been prepared for several of the common enzymes involved in the digestion of proteins, e.g., substances that catalyze the cleavage of RNA have been synthesized based upon the catalytic groups found in the enzyme ribonuclease. Mimics have also been synthesized which imitate the class of enzymes called cytochromes P-450, which are involved in many biological oxidations, and the oxygen carrier hemoglobin. Furthermore, mimics have been prepared for biological membranes and for those molecules which carry substances through membranes. These have potential applications in the construction of organized systems to perform selective absorption and detection, as in living cells.

It is important for the U.S. to build on its early lead in this field. Although most of the work mentioned above has been done in the U.S., the Japanese have also become extremely active and have specifically targeted "biomimetic chemistry" as an area of special opportunity. Research on synthetic organic chemistry develops novel methods to construct the required molecule, and elaborates new kinds of structures. The study of detailed reaction mechanisms in organic and biological chemistry permits a rational approach to catalyst design. This is an area ripe for development, deserving special encouragement as a part of this program in Chemical Catalysis.

4. *Collaboration.*

Thus, catalysis research with the four facets named here involves many subfields of chemistry (surface chemistry, solid state chemistry, organic synthesis, inorganic synthesis, photochemistry, electrochemistry, bioorganic chemistry and chemical engineering) along with the contiguous fields of solid state physics, surface physics, biology, and biochemistry. Each of these different perspectives is needed to address fully the common goal, to understand how a catalyst intermediary can enhance preferentially the rate at which a desired reaction takes place. Hence, there is great opportunity for collaboration across disciplinary boundaries.

C. *Chemistry of Life Processes*

1. *Program.*

We propose an initiative to develop and apply the techniques of chemistry and the skills of individuals knowledgeable in that discipline to the solution of molecular-level problems in life processes. This initiative includes both the application of chemical science to biology, and the development of new chemical science based on stimuli provided by biology. Research at this border between chemistry and biology requires individuals broadly competent in both areas, and a special effort must be made to develop such individuals.

The program will emphasize the molecular aspects of six areas.

- Enzymology: to understand the molecular interactions responsible for natural enzymatic activity and its inhibition; to produce natural enzymes for use in chemical synthesis.
- Immunochemistry: to learn the chemical basis of the immune and allergenic response; use, function, and modification of monoclonal antibodies; synthesis of antigens and adjuvants.
- Chemical Endocrinology: to synthesize hormones and hormone analogs; to understand hormone agonist and antagonist mechanisms.
- Neurochemistry: to determine the molecular basis of nerve transmission, neurotransmitters, agonist and antagonist chemistry, and membrane polarization.
- Membrane Chemistry and Vectorial Chemistry: to clarify active and passive transport (bioenergetics).
- Biological Model Studies: to understand host/guest chemistry, semisynthetic enzymes, and active sites.

2. *Objectives.*

- To strengthen basic research in the life sciences by providing the molecular-scale analytical, synthetic, and structural techniques required to identify, prepare, and study the organic chemical compounds which are central to modern molecular biology.
- To accelerate the conversion of qualitative biological information into techniques and substances useful in human and animal medicine and agriculture.
- To educate graduate students and postdoctoral fellows in both chemistry and biology; to provide individuals skilled in chemistry (especially organic synthesis, organic reaction mechanisms, and analytical

chemistry), who can understand and interpret biological problems and opportunities in molecular terms.

3. *Rationale.*

The study of the molecular bases of the reactions occurring in life offers enormous opportunity both for discovery in basic physical science and for application to human health, animal health, and agriculture. This area of research includes some of the most important problems which now exist in science. Solutions to these problems will have very large and beneficial impacts on society.

Biology has evolved a range of problems of revolutionary significance that now require analysis in terms of molecular interactions. The molecular synthesis and analysis required for the solutions of these problems can only be provided by chemistry.

A major fraction of biology can be reduced to two broad types of problems at the molecular level:

RECEPTOR-SUBSTRATE INTERACTIONS

Essentially all biological processes are mediated by the selective interaction of a protein receptor (enzyme, antibody, membrane and intracellular receptors) with one or more specific substrates (enzyme substrate, antigen, hormone, neurotransmitter, or simple molecule or ion).

To study these processes in molecular detail, and to control them with the precision required for rational applications in medicine, agriculture, and other areas, it is necessary to be able to:

- isolate and identify the structures of endogenous substrates or substrate analogs;
- synthesize these substrates and analogs in useful quantities and high purity;
- analyze their interactions with their receptors both in physical-chemical and biological terms;
- modify their structures to give useful agonist and antagonist activity and to facilitate effective delivery into living organisms.

The development of analytical, structural, synthetic, and mechanistic techniques appropriate to this area of molecular science represents an enormous challenge and opportunity for chemistry. The active substances may be present *in vivo* only in minute quantities; they are usually water soluble (polypeptides, polysaccharides) or surface active (lipids, membrane or hydrophobic proteins); they may have high molecular weights and complex or heterogeneous structures. Medicine and biology need the methods of chemistry to manipulate these substances; chemistry cannot presently provide fully adequate methods. Hence, the challenge and the opportunity for chemists.

MEMBRANES AND VECTORIAL CHEMISTRY

The set of chemical reactions that constitute life take place in cells and organelles. The concept of vectorial chemistry (reactions depending upon spatial separation of reactants into regions of different concentrations—that is, on concentration gradients—for their driving force) is poorly understood at a molecular level, but essential to biochemistry (the Mitchell chemiosmotic hypothesis is the best-known example).

Understanding the relations between concentration gradients across membranes and processes which form or break chemical bonds is a formidable task, one which requires active chemical modeling at both the synthetic and the kinetic level to complement the current activity in mechanistic biology. The related problem of the transport of molecules across membranes (for example, between blood and a particular type of cell) is central to the area of pharmacokinetics and drug delivery.

What reason is there to expect chemistry to be able to make progress on the many specific problems contained in these two major general classes of problems? A number of recent advances in science and engineering have provided an extraordinarily powerful set of techniques which are appropriate for the investigation of problems in chemical biology at the molecular and supramolecular level. Examples are given below.

- Recombinant DNA technology provides the opportunity to prepare proteins in substantial quantities with controlled variations in amino acid sequence.
- Monoclonal antibodies produced in large quantities using hybridoma techniques provide specific receptors against virtually any high or medium molecular weight substance.
- X-ray single crystal analysis can now solve very complex structural problems.
- Electron microscopy permits direct visualization of many structures at levels between 2 and 1000 A and is superbly suited to solving problems in membrane chemistry and in the structures of large molecules.
- Ultrasensitive analytical techniques (fast-atom-bombardment mass spectrometry, two-dimensional NMR spectroscopy, antibody-based competitive binding assays, electron capture gas-liquid chromatography, high performance liquid chromatography) can elucidate structures of small quantities of very complex substances.
- Sophisticated synthetic technology, based both on conventional chemical techniques and on a range of biological techniques, including enzymatic transformation and fermentation, make it possible to synthesize complex naturally occurring substances and analogs in useful quantities.
- Computers permit analysis of the details of receptor-substrate binding, and modeling of the complex set of coupled reactions which take place in living cells.

In summary, molecular biology has become sufficiently detailed that many of its most important current questions must be phrased and answered using chemical methods. Hence, chemical techniques are essential to understanding biological phenomena and for converting this understanding into a form useful in medicine and agriculture. There is a pressing practical reason for accelerating this application of chemistry to biological problems, namely, the economic and technological relevance of chemical biology to biotechnology and applied biology, and the intense international competition in this area. Failure to encourage the chemical aspect of biology will cost us leadership in this area and we will forfeit ownership of the practical results to other countries.

4. *Collaboration.*

An important aspect of the proposed program would be its emphasis on interdisciplinary research. Where appropriate, the program would actively encourage development of collaborative projects which integrate programs of chemical and biological research.

In addition, biotechnology is an area of extremely active industrial research. This derives from the special potential for health care (with efforts by essentially all pharmaceutical companies and by a host of small start-up biotechnology companies) and improvements in agriculture (Monsanto, du Pont, and many others). The major immediate markets being addressed by these companies are high-value proteins (interferon, plasma thrombinogen activator, insulin, serum Factor VIII, animal and human growth hormones, vaccines) and monoclonal antibody products (clinical diagnostics). Longer-term industrial projects are aimed at a range of more complex health-care products (treatments for cancer, diabetes, high blood pressure; methods for organ transplantation; immuno-regulators), improved plant strains, enzymatic catalysts for industrial and food use, biomass utilization for energy, and human genetic engineering.

The ultimate success of this industrial endeavor will depend heavily upon the supply of young scientists with the needed cross-disciplinary expertise. This program will provide such experience through research more basic than but clearly complementary to the major threads of current industrial research. For example, the development of molecular understandings of the reactions in nerve transmission and of oxidative phosphorylation are central to advances in the relevant biology but still far from application. Ultimately, these areas will be central to the development of neuroactive drugs and more efficient plants. Similarly, the development of new synthetic methods for biologically relevant molecules remains primarily an academic activity, but it is critical to the continued leadership of our pharmaceutical industry.

In fact, the scope for new research in chemical biology is so great that full and cooperative effort from both university and industry is both warranted and required. Industry is now actively building on the basic science of recent years (as well as conducting some of its own very excellent basic work); the university must provide the basic science for the next cycle of industrial discovery and development.

III. CONCLUSIONS

Chemistry extends all the way from physics, with its strong ethos of deductive logic, to the largely phenomenological biological sciences. We are at a gratifying period when chemistry is "hot at both ends." With adequate access to the powerful techniques now developing, chemistry can expect to explore and understand the principles that govern chemical change at a much more fundamental level than has been possible in the past. At this end of the spectrum, chemistry can begin to escape the bounds of empiricism imposed thus far by the intractability of many-body theory and the limits of our measurements. Yet, despite these barriers, chemists have been so enormously successful with their inductive approach that molecules of exquisite complexity can be recognized and synthesized in every intricate detail. This capability is most timely, because the phenomenological advances of the biosciences now demand explication at the molecular level. Thus, the time is ripe for quite spectacular advances in chemistry.

Hence, in the next ten to twenty years, there will be dramatic changes in our basic understandings of chemical change and our ability to marshal those understandings to deliberate purpose. The program presented here is intended to define a leadership role for the U.S., as these advances are won. The rewards accompanying such leadership are commensurate with the prominent role of chemistry in addressing societal needs, in ameliorating the problems of our technological age, and in sustaining our economic well-being. The costs of falling behind are simply intolerable.

To exploit the intellectual opportunities in chemistry and to maximize the social gain, a substantial incremental increase in federal support for basic research in the chemical sciences is needed. This need for enhanced federal investment in chemical research is rooted in a pattern of funding historically appropriate to a test-tube and bunsen burner era, an era long since eclipsed. The sophistication of a modern chemistry laboratory requires a much more vigorous and sustained financial commitment, both in capital investment and in supporting services. The cost is miniscule compared to the stakes involved; we must nurture a $175 billion industry that maintains a $12 billion positive balance of trade and employs over a million people. We must continue to provide it with a full reservoir of fundamental knowledge.

Appendix I

Fundamental Questions Before Us

A. UNDERSTANDING CHEMICAL REACTIVITY

Molecular Dynamics.

a. How is energy redistributed as a function of time if it is deposited in a molecule in a specific excitation?

b. How does the energy in a molecule (amount, states, intramolecular distribution) determine its reactivity?

c. Can the chemistry of a molecule be affected by an intense (but not absorbed) photon field?

d. Can we understand and theoretically predict the detailed energy distribution among the products in bimolecular reactions?

e. Can we observe the transition state in real time?

f. Is there a Franck-Condon aspect to H or H+ transfer?

g. How can a non-thermalized distribution of excited states be maintained and can novel chemistry be achieved thereby?

h. Can we fully characterize and understand intramolecular and intermolecular energy transfer processes?

i. Can we store solar energy using artificial photosynthesis?

j. What new reaction mechanisms operate at high temperatures because of unusual gaseous molecules and unusually rapid mobility?

k. Can we understand and predict the unusual chemical species and solid phases formed at high temperatures?

Chemical Pathways.

a. What are the systematics of the metal-ligand bond energies in organometallic compounds?

b. What are the mechanisms and rates of multielectron transfer reactions and how can they be controlled?

c. Can interfacial energy be used to synthesize new solids with unique structural features (e.g., channels, cavities, holes)?

d. How can metastable non-stoichiometric solids be prepared?

e. How can the dimensionality of a solid be controlled (linear chains, two dimensional nets, sandwich solids, etc.)?

f. What principles govern conformer-selective chemistry?

g. Can synthetic polymers that are dynamic entities be designed?

h. Can novel inorganic solids be made with molecular beam epitaxy?

i. Do topological principles underlie some aspects of chemical structures and reactions?

j. What molecular properties exhibit bistability suitable for digital information storage in a molecular electronics system?

k. Can organic ferromagnetic compounds be synthesized?

l. What are the structural requirements for nonlinear optical properties in organic molecules?

B. CHEMICAL CATALYSIS

Heterogeneous Catalysis.

a. For chemisorbed intermediate species, what are the residence times? Can they be changed to raise catalyst efficiency?

b. For chemisorbed intermediate species, what molecular structures and oxidation states give optimum selectivity?

c. Why are transition metals the best catalysts?

d. What general mechanisms determine catalyst deactivation? Specifically, how do nickel and vanadium compounds deactivate catalysts?

e. What is the combustion process of carbon on catalytic surfaces?

f. What determines surface migration of chemisorbed species on a surface? What role does this migration play in catalysis?

g. Can we identify and characterize active sites in heterogeneous catalysts?

Homogeneous Catalysis.

a. How is the rupture of H-H, C-H, and C-C bonds altered as the size of a metal cluster catalyst increases?

b. What relationships connect homogeneous, metal cluster, and metal surface catalysis?

c. Can we design homogeneous catalysts that would selectively convert coal to specific desired products?

d. How can chiral metal complexes be designed to induce chirality in organic reaction products?

e. Can we achieve selective homogeneous oxidation catalysis for terminal positions in alkanes?

f. Can catalytic Diels-Alder chemistry be developed?

g. Can oxidative fixation of nitrogen (e.g., to nitric acid) be catalyzed?

h. Can the addition of water or ammonia to olefins (to give alcohols and amines) be catalyzed?

Photocatalysis and Electrocatalysis.

a. How does catalysis at the solid-gas interface connect to electrocatalysis at the solid-liquid interfaces?

b. Can we define, control, and understand the electronic structure of surfaces?

c. What principles are involved in the design and synthesis of new electrocatalysts?

d. What principles are involved in the design and synthesis of new semiconductors materials for photoassisted reactions?

e. Can we develop analytical methods to study chemistry at the solid/liquid interface to match the power of those recently developed for use at the solid/vacuum interface?

f. How can light-absorbing dyes be chemically bound to semiconductor surfaces?

Artificial-Enzyme Catalysis.

a. What obstacles impede synthesis of artificial-enzyme catalysts tailored for a desired reaction?

b. Can we design catalysts to fix the structure (head-to-tail, head-to-head, block, etc.) and stereochemistry of polymers?

c. Can we enhance selectivity through surface shape?

d. Can artificial enzymes be designed to operate in organic solvents?

e. Can artificial enzymes be incorporated into artificial membranes to achieve energy-driven transport (as occurs in living cells)?

f. By adding binding sites for regulator molecules, can we design artificial enzymes to act as detectors? Can these be developed with feedback loops to adapt and control their environment?

C. CHEMISTRY OF LIFE PROCESSES

Enzymology.

a. What is the relation between receptor protein/enzyme binding/active site structure and specificity/catalytic activity?

b. What strategies are required to design substrates which compete with endogeneous substrate for specific receptor/active sites?

c. Can enzymes be used as practical catalysts in organic synthesis?

d. What are the mechanisms of enzymatic reactions (e.g., in protein and nucleic acid synthesis, oxidative phosphorylation, photosynthesis, active transport, intermediary metabolism)?

e. Can combined chemical/biological synthetic techniques be developed to improve markedly the synthesis of nucleic acid sequences?

f. What is the atomic-level basis for enzyme tertiary structure and stability?

Immunology.

a. What is the relation between immunoglobin structure and binding specificity?

b. What are the best techniques for producing and purifying monoclonal antibodies?
c. What antigens and adjuvants are most effective in initiating an immune response?
d. How large a fragment of a protein antigen is required to evoke an effective immune response?
e. Can monoclonal antibodies serve as a basis for chemical purification procedures? As starting materials for semisynthetic enzyme production? For new types of chemical analytical schemes?

Endocrinology.

a. What are the structures of important endogenous hormones?
b. What is the best strategy for inferring the binding specificity of hormone receptors?
c. How should one design synthetic hormone analogs that have desired activity, specificity, and *in vivo* lifetime?
d. What synthetic strategies are required to synthesize synthetic hormones and analogs (especially polypeptide hormones)?

Neurochemistry.

a. What are the structures of important neurotransmitters?
b. What related structures will have agonist/antagonist activity?

Membrane Chemistry and Vectorial Chemistry.

a. Is the chemiosmotic hypothesis correct? What is the molecular basis for interconversion of energy stored in concentration gradients and energy stored in reactive chemical bonds?
b. How is charge separation across membranes accomplished in photosynthesis, respiration, and related areas of bioenergetics?
c. What is the molecular basis for active transport processes? Can understanding of these processes be used to suggest new types of abiological membranes having useful selectivity?
d. What is the chemistry of perception (vision, smell, memory)?
e. What is the relation between chemical, physical, and biological properties of lipid membranes? Can synthetic membrane systems (liposomes, others) be developed for drug delivery?

Chemical Studies Relevant to Biological Systems.

a. Can we understand the hydrophobic effect in aqueous solutions?
b. What are the best strategies for the synthesis of water-soluble molecules having biological activity (oligosaccharides, lipids, polypeptides, neuroactive substances, nucleic acids, metabolites)?
c. What are the structural and thermodynamic bases for molecular recognition (host/guest chemistry)?
d. What are the properties of thin hydrocarbon membranes (selectivity, permeability, concentration polarization, interfacial structure, thermodynamics of membrane diffusion)?
e. How are cooperative chemical phenomena related to biological systems (liquid crystals, organized lipid assemblies, oscillating reactions, nucleation and phase transitions)?
f. Can one construct instructive chemical models for important biological phenomena (active transport, photosynthesis, oxidation phosphorylation, proton translocation, muscular contraction, information storage, nerve conduction, self-replicating systems)?

Mr. FUQUA. Thank you very much, Dr. Pimentel. We appreciate your enthusiastic report this morning. I might point out to the lady from Rhode Island that one of the things in materials that they are hoping, because of composites and so forth, is that fighter airplanes will be one-third smaller because of the less weight they have, accomplishing the same mission. We are hopeful that means one-third less cost.

Dr. PIMENTEL. There is serious talk about an all-polymer automobile, which expresses the hopes and expectations for saving cost in weight in the same way that you are talking about.

Mr. FUQUA. It is a very exciting area. You made specific recommendations as to the amount that you would add to each of the material sciences and chemical sciences subprograms at basic energy sciences. What do you think is the most important need for support: for graduate students, researchers, research instrumentation, large facilities, or repair the facilities we have?

Dr. PIMENTEL. Let me respond in connection with the chemistry of the type that I was speaking of. I believe the most important thing we should look to today is to increase the research productivity and cost-effectiveness of the research programs that we are now supporting. The funding of chemistry is based on the tradition that goes back to bunsen burners and test tubes and does not reflect the very expensive and sophisticated instrumentation I spoke to today.

I believe that the first need is to put this expensive instrumentation, in the range of $100,000 to $800,000 or $900,000 in the hands of the existing research groups that we are now supporting. The second thing that we must pay attention to is to establish in the chemistry areas that depend upon the sophisticated instrumentation the infrastructure to use it effectively. That is to say, it must not only be placed there, it must thereafter be maintained and operated by skillful people, and we do not have in chemistry the funding to provide that infrastructure. I believe that we do not need a massive increase in the number of graduate students and postdoctoral students. We need to provide them with the latest tools of their trade, the ones that industry expects them to know about when they hire them and put them to work on society's problems.

Mr. FUQUA. How much impact do you think that the briefings you gave to the various agencies had on the fiscal year 1985 budget?

Dr. PIMENTEL. I am afraid it had relatively little and probably for good and sufficient reason. The timing of our presentation at this briefing to the various agencies was determined by the timing with which Mr. Keyworth asked us to present the briefing, and that came mid-October.

Mr. FUQUA. The budget process was well on the way then.

Dr. PIMENTEL. Yes. I will say this, if you will permit me. It does seem to me that the opportunities are very great, and the amounts of money that are involved in moving forward on them in fiscal year 1985 are not so great, relative to many other initiatives that we are considering. I can tell you that the briefing report is in wide demand abroad. Every foreign visitor that comes to my office goes away with a copy of it, and I have had invitations to speak in

Sweden, in Germany, in France about it already. I have spoken in some of those places about it.

The other countries are going to pay attention to this and do something about it. I just do not think we can afford to wait.

Mr. FUQUA. Thank you.

Mrs. Schneider.

Mrs. SCHNEIDER. I wonder if you could touch on the activities in the area of liquid fuels and the development of new materials to supplant our dependence on foreign oil, based on what we just heard in the news this morning and what is going on around Lebanon and the Straits of Hormuz.

Dr. PIMENTEL. What you are asking about is very serious and important. When I spoke about the need to look for new energy sources and spoke about the decline of world production beginning around the turn of the century, that is, of course, assuming we have access. We might be denied access because of political developments, which will bring us all the more forward.

One then must begin asking the question, Where will we find alternate energy sources? Surely one of the important places that we are going to look to immediately is coal, because we have large supplies of coal. The problem, of course, is that the grade or the quality of the coal begins to decline as you begin to depend on it more and more heavily. One of the things you can do with coal is to convert it to what is called synthesis gas, which is a mixture of carbon monoxide and hydrogen. From there, you can make lots of things if you have the right catalyst, the materials that will cause reactions to proceed rapidly toward the specific desired product you want.

If, for instance, you decide that you want to go for methanol or ethanol as a major fuel replacement, you need a catalyst that will cause the materials to react. You need the right temperature and the right conditions, but most importantly the right catalyst to produce predominantly that particular material. That is one of the examples to give that really indicates the importance with getting on with advancing catalysis from this empirical state it has been into a real science. If we can design our catalyst, that will be one of the important applications.

I will just mention one more. A long-range energy source we simply cannot ignore is solar energy. So we should really have strong programs in the areas that are connected with making optimum use of solar energy. One of those, of course, is photovoltaics. But let me point out another area that deserves mention. The biomass area, in general, is one of the possibilities, and once again it is going to be necessary to understand fermentation processes. Again, we are likely to need new catalysts. We are also going to want to understand and utilize photosynthesis. This gives me an opportunity to mention that DOE has a very strong program in the plant science area also that is looking into natural photosynthesis. That is, how does the plant take the solar photon and ultimately convert it into materials of interest to us. That is a program that also deserves very strong support.

Mrs. SCHNEIDER. How anxious are you to see the United States speed up their photovoltaic program, when in fact it appears that the Japanese are considerably ahead of us and, playing devil's advocate here, might we be better off buying cheaper photovoltaics from the Japanese and investing our continuing research, for example, in something like photosynthesis development or solar power?

Dr. **Pimentel.** I certainly cannot disagree with the concept of trying to go after photosynthesis and biomass as important avenues to follow. With regard to whether we should not just buy them from Japan, my answer to that is, Let us look ahead and be the ones to bring on the next generation of photovoltaics.

Mrs. **Schneider.** To build upon what the Japanese have already achieved?

Dr. **Pimentel.** Yes. You know what the next generation of photovoltaics is going to be. It is going to be organic photovoltaics. It is not going to be amorphous silicon or gallium arsenide or whatever. It is going to be an organic material, and it is going to be as cheap as dirt, as cheap as my shirt.

Mrs. **Schneider.** Getting back to our discussion of synthetic fuels, what are your feelings insofar as essentially the lack of the private sector's willingness to take advantage of those low-interest loans made available by the Synthetic Fuels Corporation? We do not seem to see much movement in the private sector for the development of synfuels, so that leaves the responsibility essentially up to DOE. Can I rest assured that perhaps DOE is developing this, and maybe you are putting the technology on the shelf or is it a crisis?

Dr. **Pimentel.** I am not able to make an answer to the last part of the question, Is DOE going to have this in hand or not. I would make the remark that what has happened over the last 3 years or so, in reference to the oil glut, which we are all aware of by watching the price of gasoline go up to $1.50 and now it is back down around $1 a gallon in California. You wonder what on earth is going on there. Well, there are complicated economic factors that are involved. One of the things that happened was that as the price of gasoline and fuel went up, people began converting to coal in industrial use, and people like you and I began watching how many gallons of gas we spent, and use went down—so much that our refining capacity momentarily was able to get ahead. So we have a momentary glut.

As the price goes down, the investment that any industry is willing to make into an alternate energy source whose economics is predicated on high prices of gasoline for competitive fuel, of course——

Mrs. **Schneider.** If you'll excuse me for interrupting, I think the point the Chairman and I were trying to make was——

Dr. **Pimentel.** I think that the forces that you refer to are sufficiently capricious that it might well be that we want to put some stability in the program of this sort by guaranteeing that it moves ahead in spite of such capricious things. And that suggests to me that DOE might well have a role in the synfuels program to keep it moving ahead.

Mrs. **Schneider.** OK.

Dr. **Pimentel.** Which I think is the question that you were asking.

Mrs. **Schneider.** Right. Exactly. And considering we have the Synthetic Fuels Corp. with, I guess; $16 billion sitting there off budget and not really being used, would you be supportive, due to the lack of interest on the part of the private sector for the development of synfuels, perhaps earmark some of those moneys for other energy technologies such as trash to energy, or district heating and cooling?

Dr. PIMENTEL. You're getting beyond my expertise in asking about how those particular allocated funds might be diverted to other purposes. The programs that you speak of, I'm surely for; whether that's the appropriate way to fund that system, I'm not able to say.

Mrs. SCHNEIDER. Do you think that biomass could be stimulated through that kind of loan guarantee?

Dr. PIMENTEL. I would expect so, but I really do not want to claim to be an expert in that particular—you're talking about how the Government can interact with industry to stimulate desired ends, and that just gets beyond my particular expertise.

Mrs. SCHNEIDER. OK. Over the last 3 years our committee has seen the reduction in the funding for a number of R&D programs in the alternative energy area, and I'm curious to know whether you feel there ought to be more opportunities for demonstration projects so that the private sector could take advantage of pilot project opportunities. Do you think that that's a worthwhile area of pursuit for the private sector?

Dr. PIMENTEL. Well, I have really addressed most of my concern and comments today about what I would term the longer range research programs of DOE and how DOE can look ahead to the future of the country and the welfare of the country some 10 or 20 years away. I think you're asking a question now of a shorter range type, and I guess I just have to say that you're into an area where we're not talking so much about scientific issues as, what is the optimum political approach to a particular problem of society. And my answer would be entirely a personal one; I can understand the arguments on both sides, one saying that if industry will do it, let's let them do it and encourage them; and on the other side—but on the other hand, can we afford for them possibly not to do it? And I say, I think this is in the political arena where you'd only be hearing one person's private opinion.

Mrs. SCHNEIDER. Well, I thank you for that. I am interested in this one person's political opinion; and having the scientific involvement that you have would certainly help us to make better political decisions ourselves. But I thank you for your testimony today; I found it most enlightening.

Thank you, Mr. Chairman.

Mr. FUQUA. Thank you very much. Thank you, Mrs. Schneider, and Dr. Pimentel, thank you very much for being with us today.

Dr. PIMENTEL. This was so you could tell I'm a chemist, in case it didn't come through in my testimony.

Mr. FUQUA. Maybe the other disciplines might want to ask equal time. [General laughter.]

But you'd be a hard act to follow.

Our next panel, on the Center for Advanced Materials includes Dr. Albert Narath, executive vice president, Sandia National Laboratories in Albuquerque; Dr. Peter Eisenberger, director of the Physical Sciences Laboratory, Exxon Research & Engineering Co.

from New Jersey; Dr. M. L. Knotek, Surface Science Division, Sandia National Laboratories in Albuquerque; and Dr. Hermann Grunder, associate director, Accelerator & Fusion Research Division, Lawrence Berkeley Laboratory, and Dr. Gabor A. Somorjai, Center for Advanced Materials, Lawrence Berkeley Lab.

As we have indicated to the other members, if you wish to summarize your statements and place the prepared remarks that you have into the record, that permission is granted.

If the light's on, it's working.

Dr. Narath, we're very pleased to hear from you first.

STATEMENT OF DR. ALBERT NARATH, EXECUTIVE VICE PRESIDENT, SANDIA NATIONAL LABORATORIES, ALBUQUERQUE, N. MEX.

Dr. Narath. Thank you, Mr. Chairman, members of the subcommittee.

I'm pleased to appear before you today to discuss what is now a page of the history book, specifically I'm here to summarize for you the findings and conclusions of an ad hoc panel which Dr. Trivelpiece asked me to chair last year. The task assigned to us was to conduct a technical and programmatic review of the Lawrence Berkeley Laboratory proposal for a National Center for Advanced Materials, so-called NCAM. The panel was asked to examine all the elements and activities proposed for the center including a review of the proposed facilities, organizational arrangements, and other related matters. The deliberations of the panel were constrained on only two points: one, the choice of materials science as the topic for a new DOE National Laboratory initiative, and two, the selection of LBL as the location for that initiative.

The panel submitted a final report to the DOE on August 31, 1983, at which time the panel disbanded.

I have no detailed knowledge of subsequent NCAM developments, and will therefore limit my remarks to a brief summary of the panel's principal conclusions as contained in its final report.

I have provided this subcommittee a more complete written statement which includes a listing of the panel membership and a full account of its findings.

As you recall, the materials center proposed by LBL was first described in its fiscal year 1983 institutional plan, and featured a vacuum ultraviolet/soft X-ray synchrotron radiation source, the ALS, as the centerpiece of an expanded LBL materials R&D effort with emphasis on increased industrial participation. In addition to the ALS, the proposal requested several other major construction line items and associated operating and equipment funds. The line items were the Surface Science and Catalysis Laboratory, Advanced Materials Synthesis Laboratory, and finally, Advanced Device Concepts Laboratory.

In addition, the NCAM proposal included funding for improvements at the Stanford Synchrotron Radiation Laboratory, SSRL.

Now, to provide a framework for its deliberations and to guide its review, the panel adopted a set of criteria which are consistent, we believe in general terms, with recommendations of recent DOE laboratory studies conducted by the DOE Energy Research Advisory Board and the White House Science Council. Let me mention these criteria rather quickly: first, relevance to an advanced materials theme; two, realistic potential for significant impact on important U.S. industries; three, program goals and objectives whose attainment requires centralization of research effort; four, contribution to a new or strengthened mission for LBL; and finally, five, resource requirements not excessive in relation to value of projected accomplishments.

On balance, the panel concluded that the establishment of a materials research center at LBL offers exciting opportunities for significant advances in this technologically important field. This conclusion was based in large measure on the excellence and vigor of LBL's Materials and Molecular Research Division, MMRD, program in materials science and related topics. You may know that the MMRD professional staff includes a large number of University of California faculty; at the time of our review, some 140 postdoctoral and visiting scientists; and almost 400 graduate students. Because of the stringent faculty screening process, the MMRD staff represents an unusually talented and productive group of investigators. Not surprisingly, given the strong integration of LBL and University of California research activities, the program consists of a large number of essentially uncoordinated, small scale investigations covering a very broad range of subjects, not unlike typical university programs. Such an approach is, unfortunately, not consistent with the review criteria which the panel established. The proposal was therefore judged to require substantial alterations to assure four things.

First, a structured "technology-pull" orientation which complements and builds on existing "basic-research-push" programs at Berkeley.

Two, selection of a limited set of topical areas of industrial importance.

Three, a directed research approach which encourages individual innovation while pointing the collective effort toward clearly defined goals.

And four, and very importantly, implementation of close contacts with industry.

In our view, by far the most serious inconsistency in the proposal was the combination of materials R&D and the ALS in a single initiative. Judged in terms of its potential contribution to a goal-oriented, "technology-pull" materials theme, the ALS would require a disproportionately large share of NCAM resources. The resulting program imbalance makes the ALS an inappropriate centerpiece for such an enterprise.

The panel concluded that the two NCAM components should, therefore, be divorced from each other and considered separately on their own merits.

The materials R&D component which in recent times, I believe, has been referred to as CAM, was in our view the essential part of the LBL initiative based on the stated goals of the enterprise. And in our view should be characterized by a technology focus. The ALS, on the other hand, should be regarded as a major user facility in the traditional sense.

While the panel favored continued support for R&D on advanced light sources at LBL, it was not in a position to judge the merit of the ALS in competition with other major facility interests of the Nation. The panel felt, instead, that the decision whether or not to proceed with the ALS should await completion of a review by the synchrotron radiation community.

I might mention that the proposed upgrade of the SSRL facility was strongly supported by the panel, largely because of the leverage provided by even modest incremental investments at this existing facility.

But turning quickly to the materials initiative, let me say that the panel concluded that several actions should be taken expeditiously to insure that CAM is pointed in the proper direction from the outset. Successful realization of CAM would result in an activity with the following dominant characteristics: one, the organization would seek major contributory roles in a few selected areas, and not simply augment or slightly extend the materials R&D efforts now performed elsewhere; two, programs would be supported based on their direct relevance to either major industrial technologies that are now or will in the future be limited by available materials, or strategic-materials interests of the Nation which are not being addressed by the private sector; three, the organization would serve as a link between appropriate National Laboratory and industrial communities, on one hand, and between academic and industrial communities on the other; and four, program planning and execution would involve significant direct participation by the industrial community, including the commitment where possible of R&D funds for joint efforts.

To be more specific, among the three broad materials areas described in LBL's NCAM scientific program summary, the surface science and catalysis activity was judged by the panel to be the strongest, primarily on the basis of the quality and breadth of LBL's ongoing catalysis research. The panel strongly endorsed construction of the Surface Science and Catalysis Facility beginning in fiscal year 1984. In regard to the other two areas, advanced materials synthesis and advanced device concepts, the panel concluded that final judgement of these activities should be delayed until an acceptable CAM program plan is available for review. Construction of the associated facility should, of course, be deferred until that time.

In closing, let me remark that the panel viewed CAM, if implemented successfully, not only as a measurable redirection of LBL, but also—and perhaps more importantly—as a serious attempt to pioneer a new mode of materials research in a DOE national laboratory. How useful the experience gained in establishing CAM will be to other laboratories, of course, remains to be determined. The close association of LBL with UC-Berkeley creates opportunities as well as problems which are not, in most instances, encountered by other Federal laboratories. For example, the major university setting of LBL offers outstanding opportunities for technical interactions with world-class scientific talent. On the other hand, CAM is likely to encounter staffing and management problems which would be much less serious at laboratories where traditions are more closely related to industrial models.

Nevertheless, the panel viewed CAM as an enterprise deserving of strong encouragement and support.

At this point I would be happy to answer any questions you may have, or wait until the other panel members have made their presentations.

[The prepared statement of Dr. Narath follows:]

Statement of Albert Narath
Executive Vice President
Sandia National Laboratories

Subcommittee on Energy Development and Applications
of the
House Science and Technology Committee
February 23, 1984

Mr. Chairman and Members of the Subcommittee:

I am pleased to appear before you today to discuss the findings and conclusions of the *ad hoc* Panel which was appointed in late March 1983 by Dr. A. W. Trivelpiece, Director, Office of Energy Research, Department of Energy (DOE), to conduct a technical and programmatic review of the Lawrence Berkeley Laboratory (LBL) proposal for a National Center for Advanced Materials (NCAM). The membership consisted of A. Narath (chairman), D. R. Davies, J. M. Deutch, J. L. Doyle, F. R. Gamble, Jr., K. L. Kliewer, J. A. Krumhansl, D. W. Lynch, W. D. Nix, H. W. Paxton, D. A. Pistenmaa, P. E. Seiden, H. G. Stever, and D. K. Stevens (executive secretary). The Panel was asked to examine all the elements and activities proposed for the Center including a review of the proposed facilities, organizational arrangements, and other related matters. The NCAM initiative was intended to be responsive to DOE's commitment to directing its Laboratories' efforts into more productive areas, especially in regard to their interactions with industry. The deliberations of the Panel were therefore constrained on only two points: (1) The choice of materials science as the topic of a new DOE National

Laboratory initiative, and (2) the selection of LBL as the location for the initiative. The initial meeting of the Panel took place April 22-23, 1983 at LBL, an interim report was provided June 10, 1983, and a final report was submitted to the DOE August 31, 1983, at which time the Panel disbanded. Since I have no detailed knowledge of subsequent NCAM developments, I will limit my remarks to a summary of the Panel's principal conclusions as contained in its final report.

The Materials Center proposed by LBL, as first described in its FY 83 Institutional Plan, featured a VUV/soft x-ray synchrotron radiation source (ALS) of superior characteristics (in terms of brilliance and time structure) as the centerpiece of an expanded LBL materials R&D effort with emphasis on increased industrial participation. In addition to the ALS, the proposal involved several other major construction line items:

(1) SSCL - Surface Science and Catalysis Laboratory
(2) AMSL - Advanced Materials Synthesis Laboratory
(3) ADCL - Advanced Device Concepts Laboratory
Functions (2) and (3) would be combined in a single laboratory building.

In addition, the NCAM proposal included funding for improvements at the Stanford Synchrotron Radiation Laboratory (SSRL), namely SEPFF - Stanford Extended Photon Flux Facility.

Review Criteria

As a starting point for the deliberations the Panel kept sight of the following DOE objectives: (1) To treat the National Laboratories as institutions rather than sites where unrelated technical work is performed and to seek new missions where necessary to assure their continued vitality. (2) To redirect, where necessary, Laboratory efforts into areas of greater relevance to national needs, both scientifically and technologically. (3) To define new modes of enhanced interaction among the Laboratories, industry and universities.

The Panel also believed that an urgent need exists in the U.S. to accelerate the translation of basic knowledge into new technology. A more rapid and efficient transition between results of basic research and industrial applications remains a major challenge for the scientific community. More effective coupling mechanisms between research and development, as well as practical approaches to improved selectivity in the pursuit of new knowledge are among the important issues which have generated considerable discussion. The Panel noted that the prospects for achieving significant near-term gains are especially encouraging for materials science. First of all, it is a subject of great industrial importance because of the essential and often limiting role of materials in modern technology. Moreover, advances in the state of knowledge in supporting scientific disciplines such as condensed-matter physics and chemistry, as well as relevant engineering disciplines, offer growing opportunities for the development and utilization of advanced materials. Underlying its subsequent conclusions, the Panel made the reasonable assumption that a materials research program directly aimed at contributing to the crucial knowledge-to-application transition can form the basis for a DOE mission assignment. The Panel also recognized that the materials field is extremely broad and diverse. Any individual program or laboratory focus can at best address only a small segment of the subject, making thoughtful selection of topics an essential requirement.

Guided by these considerations, the Panel decided to evaluate the NCAM proposal according to criteria which can be represented qualitatively by the following set of desired attributes:

(1) Relevance to an advanced-materials theme

(2) Realistic potential for significant impact on important U.S. industries, consistent with established policies regarding federal laboratory/industry interactions and DOE responsibilities.

(3) Program goals and objectives whose attainment requires centralization of research effort.

(4) Contribution to a new or strengthened mission for LBL, justifying the claim of a laboratory redirection.

(5) Resource requirements not excessive in relation to value of projected accomplishments.

Findings

(A) General Observations

It was the opinion of the Panel that the NCAM proposal, considered in detail, did not adequately satisfy the criteria listed above. Nevertheless, the Panel concluded that the establishment of a materials center at LBL offers exciting opportunities for significant advances in this technologically important field. [This conclusion is based in large measure on the acknowledged excellence and vigor of LBL's MMRD (Materials and Molecular Research Division) program in materials science, and related topics. The MMRD professional staff includes more than 50 University of California (UC) faculty, 140 postdoctoral and visiting scientists, and 360 graduate students. Because of the stringent faculty screening process, the MMRD staff represents an unusually talented and productive group of investigators. Not surprisingly, the program consists of a large number of essentially uncoordinated, small scale investigations covering a very wide range of subjects, not unlike typical university programs.] Realization of these opportunities, however, requires substantial alterations of the original proposal to assure that:

(1) a structured "technology-pull" orientation is achieved which complements the more traditional unstructured "basic-research-push" orientation of LBL's MMRD;

(2) careful selection of a limited set of topical areas is accomplished, which build on existing MMRD and/or university strengths at Berkeley and are of demonstrable interest and importance to the concerned segments of the industrial community;

(3) the research is tightly structured, and directed in such a way as to encourage individual innovation while maximizing constructive interactions among the various activities. At the same time the collective effort should be pointed toward clearly-defined and understood goals and objectives. It is this combination of features which distinguishes those large-scale materials research efforts, e.g., Bell Laboratories, which have consistently achieved significant impacts on technology. Realizing such collective effects demands a centralized organizational arrangement as envisioned for NCAM;

(4) procedures are implemented to maintain close contacts with industry in regard to program definition, priorities, execution, and termination as appropriate.

The Panel concluded that the proposal exhibits a major flaw by combining two weakly related and mutually interfering components in a single package -- namely materials R&D and the

ALS. The Panel fully recognized that synchrotron radiation has become an important research tool in materials science, as it has in other fields. Nevertheless, judged in terms of its potential contribution to a goal-oriented, "technology-pull" materials theme, the ALS requires a disproportionately large share of NCAM resources. It is therefore an inappropriate centerpiece which causes an unacceptable program imbalance.The materials component suffers loss of credibility because the ALS is a heavy burden which would inevitably divert NCAM resources and management attention. In fact, it is likely that the materials program would in time become captive in substantial measure to technical challenges facing development and operation of the ALS, instead of the ALS supporting the materials initiative, as proposed. Failure to establish the recommended industrially-motivated technology focus is therefore almost assured at the outset.

By this line of reasoning the Panel was led to the conclusion that the two principal components of NCAM should be decoupled and each considered on its own merits. In other words

NCAM ⟶ NCAM' + (ALS + SSRL improvements)

with the materials component NCAM' being characterized by a technology focus, and the ALS (and SSRL) by a user-facility focus in the usual sense. In the meantime LBL has adopted the title Center for Advanced Materials (CAM) for the NCAM' component and I shall use this designation in the following discussion in order to avoid confusion.

(B) Materials Initiative (CAM)

The materials program described in the NCAM Scientific Program Summary is organized around the three laboratories, SSCL (Surface Science and Catalysis), AMSL (Advanced Materials Synthesis), and ADCL (Advanced Device Concepts). Among the three areas, the Surface Science and Catalysis activity was judged by the Panel to be the strongest, primarily on the basis of the quality and breadth of LBL's on-going catalysis research. The Panel also regarded this area as technologically extremely important and promising, and therefore an appropriate choice for increased support. For these reasons, the Panel strongly endorsed construction of the SSCL facility beginning in FY-84. This laboratory was authorized several years ago. Although the Panel was convinced that an expanded effort in the Surface Science and catalysis area at LBL is fully justified, it remained for LBL to complete a coherent plan which is in harmony with CAM objectives.

The catalysis area is one in which industrial participation may be especially difficult to achieve because of the sensitivity of most U.S. industrial concerns to catalysis-related proprietary rights and trade secrets. If mechanisms for effective cooperative efforts are found in this area they should be easily adaptable to other CAM programs. In this regard it is noteworthy that several of the LBL scientists have extensive experience in major industrial laboratories active in catalysis.

In regard to the two other areas, Advanced Materials Synthesis and Advanced Device Concepts, the Panel believed that final judgment of these activities should be delayed until an acceptable CAM program plan is available. Construction of the AMSL/ADCL facility should therefore be deferred until a subsequent review of that plan has been completed. The Panel questioned whether organizing materials synthesis as a separate, programmatic activity is wise. The same concern applies to the device activity. It is likely that integration of these activities into other CAM programs will be found advantageous. However, the Panel also recognized that innovative research in chemical synthesis and related activities (i.e., the creation and subsequent characterization of novel, potentially useful materials) is not always most productive under the pressures of a directed program. Because of the critical role of new materials in an advanced-materials program, it is highly desirable that balance be maintained in materials-synthesis research. For this reason the Panel suggests that LBL consider strengthening the materials-synthesis effort in the MMRD, consistent with CAM growth. The contributions to future CAM programs which may be anticipated from this action provide an illustrative example of benefits resulting from interactions between the MMRD and CAM. Interactions of this type between the two organizations will also increase the contact between CAM and the local educational enterprise because of the large fraction of faculty and students associated with the MMRD, a relationship which will surely continue.

The Panel concluded that several actions should be taken expeditiously to assure that the materials initiative is pointed in the proper direction from the beginning.

(1) The goals and objectives of the materials initiative should be restated by LBL to clarify its intended technology focus. Included in this statement should be mention of the ALS decoupling.

(2) A CAM Director should be appointed as soon as a strong candidate can be identified. The individual chosen

for this position must have a thorough understanding of the industrial community and its needs, have experience in managing directed research, and possess requisite scientific credentials. The Director should not be made responsible for ALS planning or operation.

(3) A CAM advisory board should be organized, with strong industrial representation, to provide policy guidance.

(4) An acceptable CAM program plan should be developed under the CAM Director's guidance. This process should begin with a systematic identification of major industrial activities which are seriously constrained by available materials technology.Before any commitments to specific topical areas are made, contributions to the national effort by existing programs at other institutions should also be carefully weighed. To the maximum extent possible CAM should strive to develop major roles in a few, carefully chosen, technologically important areas of materials science in which the current national effort is demonstrably inadequate.It is most essential that this planning effort involve strong industry participation.

(5) An organizational structure should be established which fits the CAM program objectives. This task should include the definition of an appropriate CAM/MMRD interface to assure an effective functional relationship between these organizations. In this connection, careful thought should be given to the possibility of transferring some existing MMRD activities to CAM in order to expedite the start-up phase of the new initiative. The Electron Microscopy Center is an example of an MMRD activity which might be examined for possible assignment to CAM.

(6) Effective mechanisms for industrial involvement should be implemented. The desired close coupling to the industrial community poses a major challenge and may require organizational concepts and procedures (e.g., funding schemes) not part of LBL's tradition. Existing models which have proven effective elsewhere should be examined for CAM applicability. Among relevant DOE examples, the Sandia Combustion Research Center may be cited; possible university examples include Stanford's Center for Integrated Systems (CIS) and Cornell's National Research and Resource Facility for Submicron Structures (NRRFSS). Careful thought should be given at the outset to matters related to patent rights and proprietary information. Every effort should be made to avoid unnecessary disincentives in this regard for industry involvement in CAM research programs. Consideration should also be given to joint DOE/industry funding for appropriate project efforts.

(7) A funding strategy should be developed. Special consideration should be given to integration of ER/BES funding with support from DOE's programmatic organizations (i.e., nuclear, fossil, solar, etc.), as well as industry. Such augmentation of BES resources would strenthen the technology focus and promote more effective program balance between fundamental and applied research. It would also assure that the program objectives remain consistent with DOE's mainline responsibilities, thereby strengthening the CAM claim to a DOE mission designation. Nevertheless, a single program office in DOE should be given oversight responsibility for CAM, together with the

requisite authority to prevent destabilizing effects of multiple funding sources and to assure balance and cohesion among various program elements. Since the core effort will be funded by the Materials Sciences Directorate of BES, that office is the appropriate choice for this assignment.

(8) A staffing strategy should be developed. The Panel viewed staffing to be a critical obstacle to successful implementation of the CAM concept. A highly motivated, technically superior professional staff is essential. The excellence of the MMRD is built largely (though not entirely) on UC faculty. Unfortunately, this LBL tradition will not serve the CAM needs. In the first place, only a limited number of faculty appointments will be available in the near term to support CAM growth. In the second place, it is highly doubtful that a directed, goal-oriented program as described here can be conducted with a staff which is dominated by university faculty, students and postdoctoral fellows. A major challenge will therefore be to attract and retain a sufficient number of senior staff without the inducement of faculty appointments. The Panel hopes that staff additions for CAM programs can be satisfied to a large extent by outstanding individuals sufficiently early in their careers that faculty appointments are not likely to be a significant issue. The Berkeley reputation for scientific excellence should be helpful in recruiting such first-rate talent. Nevertheless, the creation of a climate at LBL in which professional status in the materials-sciences field is not equated to faculty appointments must be viewed as a fundamental management problem.

(C) ALS and the SSRL Improvements

The Panel recognized the important role of synchrotron radiation in a wide variety of scientific investigations. Indeed, it is expected that advanced light sources with higher brightness and different time structures will be required for future research. However, the ALS was not judged by this Panel to be an appropriate centerpiece for an advanced materials initiative. Rather, it should be considered on its own merits. The Panel felt that an evaluation of the ALS based on broader user interests requires a separate review involving the national synchrotron radiation community, especially since the Panel was not in a position to take a definitive stand on three crucial issues affecting the ALS decision:

(1) Urgency of another synchrotron source at this time.
(2) Choice between VUV and hard x-rays for the next light source.
(3) Near-term technical feasibility of a light source capable of attaining the specified ALS operating characteristics in a reliable, reproducible manner.

As concerns the time-urgency question, the Panel believed that the argument revolves less around the need for an increased number of synchrotron-radiation beam lines than around the increased utility of synchrotron radiation with qualitatively different characteristics -- in the present case, significantly shorter pulse durations and/or higher spectral brightness. History suggests that new measurement capabilities usually stimulate unexpected scientific advances. The value judgment should, of course, be left to the user community.

If a decision is made subsequently to proceed with an advanced VUV/soft x-ray facility, its location at LBL would be a sound choice. The following considerations contributed to this view:

(1) LBL's record of accomplishment in the development of insertion-device technology.

(2) LBL's outstanding accelerator science and engineering staff.

(3) The assured availability of LBL support facilities.

(4) A west coast location of a major VUV/soft x-ray facility would contribute a greater geographic balance to the national synchrotron effort; with the complementary SSRL emphasis on hard x-rays, a balanced west coast synchrotron user complex would be created.

Regardless of when or how a final decision on the ALS is reached, LBL should continue to pursue the following tasks:

(1) Since the ALS represents an advance in electron storage-ring technology and will produce synchrotron radiation with very high spectral brightness and very short pulse lengths, additional facility R&D is desirable to minimize design uncertainties. This includes design studies on insertion devices, optical materials and components, and the proper choice of vacuum-tank material. Short-bunch-length phenomena should be studied. Also, the impact of the proposed superconducting wiggler on the performance of the other insertion devices should be evaluated further.

(2) Develop a broader community of potential users and quantify their needs.

(3) Explore design alternatives aimed at lower cost, and greater responsiveness to user community interests as judged by past workshops and future interactions.

All of these activities are of considerable general interest, and promise to benefit the future of synchrotron-radiation research independent of the ALS decision. The Panel believed that support should therefore be provided for the above mentioned activities.

Should the ALS or a similar facility be located eventually at LBL it would require a resident, core research program for its effective operation as a user facility. Resources for such an activity should not be drawn from CAM funding, except to an extent clearly justified by CAM program interests. The Panel recognized that LBL and SSRL both have strengths in the synchrotron-radiation area. Cooperation between these institutions has contributed significantly to capabilities and accomplishments of the SSRL facility. Both groups would benefit from further strengthening of their collaborative efforts, especially in connection with plans for future facility additions and improvements at the two locations. In the meantime, the proposed upgrade of the SSRL facility was strongly supported by the Panel. This support was based on the following reasons:

(1) Within the constraints imposed by current facility limitations, SSRL has established an extensive user community (with participation from industry, universities, and other laboratories), and can point to significant scientific accomplishments.

(2) The existing support facilities at SSRL are marginal in relation to existing needs and opportunities.

(3) Currently available high-quality beam time at SSRL is inadequate to meet user demands.

(4) The opportunity exists to install a hard x-ray beam line of superior characteristics on PEP at relatively modest cost.

Concluding Remarks

Successful realization of CAM as viewed by the Panel would result in an activity with the following dominant characteristics:

(1) The organization would seek major contributory roles in selected areas and not simply augment or slightly extend the materials R&D efforts now performed elsewhere.

(2) Programs would be supported based on their direct relevance to either major industrial technologies that are now or will in the future be limited by available materials, or strategic-materials interests of the nation which are not being addressed by the private sector.

(3) The organization would serve as a link between appropriate National Laboratory and industrial communities, on one hand, and between academic and industrial communities, on the other.

(4) Program planning and execution would involve significant direct participation by the industrial community, including the commitment of R&D funds to joint efforts.

Decisions concerning future growth and maximum size of CAM should be based on LBL's progress toward establishing programs having the recommended character. Assuming complete success, the Panel envisioned an CAM enterprise comprising a total technical staff of perhaps a few hundred at steady state, requiring an annual operating budget (derived from several sources) in the range of $30-50M. This estimate was derived from experience with comparable directed-research activities at other institutions and the expectation that a successful CAM would eventually develop 2-4 areas of concentration in addition to the initial catalysis effort. Because of the subjective nature of these considerations, the size projection is, of course, subject to some uncertainty. An effort of this magnitude would constitute a measurable redirection of LBL and would also be of sufficient magnitude to qualify the activity as a serious attempt to pioneer a new mode of materials research in a DOE National Laboratory. How useful the experience gained in establishing CAM will be to other laboratories, however, remains to be determined. The close association of LBL with UC/Berkeley creates opportunities, as well as problems, which are not in most instances encountered by other federal laboratories. For example, the major-university setting of LBL offers outstanding opportunities for technical interactions with world-class scientific talent. On the other hand, successful implementation of CAM at LBL is likely to encounter staffing and management problems peculiar to that institution. These would be much less serious at Laboratories where traditions are more closely related to industrial models.

The FY-85 funding requirements include construction funds to assure rapid completion of the SSCL and SSRL/SEPFF projects, as well as adequate operating and equipment funds for development of advanced synchrotron-radiation technology and CAM research. However, whether commitment of design funds for the AMSL/ADCL facility will be justified in FY-85 could not be determined by the Panel at the time of its deliberation. The Panel concluded that a final decision should be contingent on progress by the CAM team , especially in regard to program planning.

Mr. **Fuqua**. I think we'll wait until the other panel members have presented their testimony and then we'll have questions of all of you. Thank you.

Dr. Eisenberger.

Dr. **Eisenberger**. Dr. Knotek will address you first.

Mr. **Fuqua**. OK. Thank you.

STATEMENT OF DR. M. L. KNOTEK, SURFACE SCIENCE DIVISION 1134, SANDIA NATIONAL LABORATORIES, ALBUQUERQUE, N. MEX. AND DR. PETER EISENBERGER, DIRECTOR, PHYSICAL SCIENCE LABORATORY, EXXON RESEARCH & ENGINEERING CO.

Dr. **Knotek**. I'd like to request that our report and the summary of comments here be entered in the record.

Mr. **Fuqua**. Yes. We will do that for all the panelists.

Dr. **Knotek**. Thank you, Mr. Chairman, and members of the subcommittee. It's a pleasure to have the opportunity to come before you to summarize the results of our study on advanced national synchrotron-radiation facilities.

The task of our committee was to assess the future opportunities and technical needs for synchrotron-radiation-based research and technology in the United States. Our committee consisted of 17 members, including 12 users of synchrotron radiation. We met on 4 separate occasions including a meeting which involved 80 participants and 30 speakers, including users, representatives of the facilities, and others. As the study proceeded we issued additional calls for letters of opinion and for technical and factual information. Over 100 such correspondences were received, and over 1,000 pages of written technical information were supplied to our committee. In addition, we were in constant contact with many members of the community for advice and technical discussions.

In our study we evaluated the current status and future prospects for synchrotron-radiation-based science and technology, the facilities, and the users. Our judgments were based on the new science and technology offered by the next generation of sources, and the way in which the properties of the new sources lead to new capabilities.

Our recommendations for synchrotron radiation include upgrading of existing facilities, new instrumentation, new facilities, and methods of increasing user participation, especially by applied interests. Our full report is now ready and available for this committee.

Throughout the development of modern science and technology, light has been the most effective and versatile of probes for the discovery of structural characteristics and for the understanding of physical processes. The frontiers of science have been intimately linked to the evolution, the revolution, and the technology of radiation generation like the mercury lamp, the X-ray tube, and the laser.

Synchrotron radiation produced by electron storage rings is very intense throughout the range provided by all previous sources. The first introduction of synchrotron radiation in the late 1960's provided orders of magnitude gain in intensity over other sources in the ultraviolet and X-ray regions. This set off a revolution in the use of radiation to probe materials and phenomena. The implementation of a new generation of dedicated machines, the National Synchrotron Light Source at Brookhaven and the Synchrotron Radiation Center at the University of Wisconsin which are especially configured to produce a bright source, is leading to further improvement.

Now, within the last few years we have become confident that a new generation of synchrotron radiation facility can be built that will provide a gain in source properties as revolutionary as the original introduction of synchrotron radiation. To fully exploit this new technology, a new generation of machines must be designed and built. And this has launched new initiatives for facility development.

This new technology is based on new types of magnetic structures, called wigglers and undulators which are inserted into long, straight sections of storage rings to produce extremely bright and controllable radiation beams. The current generation of storage rings is not designed for insertion devices and contains only limited opportunities for them to be utilized. The new generation machine will be designed especially for their use. The physics of these devices dictate that to optimize performance through the whole spectrum, two machines are necessary.

The use of storage rings as sources of radiation is not limited to this country. Synchrotron radiation science has had a similar impact on the industrialized countries of Europe and Asia. All of these countries expect industrial and defense applications to grow rapidly in significance, and are building an array of synchrotron radiation facilities to handle the work. In West Germany, France, England, the Soviet Union, and Japan, there are synchrotron radiation facilities comparable to those in this country, and these countries all have high-priority programs to advance their capabilities, including the utilization of this new technology.

In the brief history of synchrotron-radiation-based science and technology and research there have already been many significant accomplishments in a wide variety of fields. Fundamental new capability has been provided in the studies of solid state physics, surface science, chemistry, biology, medicine, energy research, and materials research. While the thrusts to date have concentrated on the basic sciences, synchrotron radiation is taking on an increasing relevance to technology and security applications. Synchrotron radiation has been applied to catalysis and the identification of impurities in coal, particularly relevant to Dr. Pimentel's presentation. They have been applied to submicron lithography for the computer industry, the study of materials properties important to various manufacturing industries such as steel, as well as the study of biological materials and such things as medical imaging, where noninvasive, low-dose angiography techniques have now been developed.

With the new generation of sources one sees expanding horizons of experimentation in all these areas, together with increased usage of the present techniques with greatly expanded capabilities by a larger number of researchers and engineers. The scientific and technological impact will be greatly expanded and will provide innovation affecting a broad range of industrial and strategic interests.

To meet the challenges and opportunities in synchrotron radiation, facilities will be needed which are dedicated to the utilization of insertion devices and are readily accessible to the whole spectrum of science, technology, and defense interests. Such new facilities, even if they are developed on the most expeditious schedule, will not have significant impact until the late 1980's or early 1990's. For this reason we need to proceed now to develop this capability, both by the construction of new facilities and by development of existing insertion-device potential to the extent possible on existing facilities.

On the basis of all the above factors and others too technical to describe here today, the committee has arrived at the following unanimous recommendations.

Regarding existing facilities and projects, the committee recommends that steps be taken to insure the timely completion of the commissioning of the National Synchrotron Light Source at Brookhaven National Laboratory and the Synchrotron Radiation Center at Stoughton, Wis. We are encouraged by the actions of these facilities since our initial letter to the Department of Energy. To optimize utilization of existing facilities, we recommend providing operating funding so that such facilities can provide a maximum of beam time in a user friendly mode, and continued research funding so that it will be possible to take full advantage of the facilities.

To realize the full potential of existing facilities, the committee recommends expeditious completion of currently approved projects to construct insertion-device beamlines: the NSLS phase II project at Brookhaven National Laboratory, and the SSRL enhanced photon flux facility project at Stanford, in particular. The future construction of additional insertion-device-based beamlines at existing facilities is strongly recommended.

Regarding major new facilities, the committee believes that major new programs based on the utilization of insertion devices are of central importance for effective progress in materials science, physics, biology, and chemistry research over the next decade. The committee is therefore unanimous in its recommendations, which follow in order of priority.

One, the design and construction of a high-energy storage ring capable of providing fundamental undulator radiation in the X-ray region of the spectrum up to 20 kiloelectronvolts, with an early 1990's target date for full operation of the facility. To achieve this objective, appropriate research and development funding should be allocated now.

Two, the construction of a second, lower energy ring capable of providing fundamental undulator radiation in the soft X-ray region of the spectrum up to 2 kiloelectronvolts. This machine should also provide picosecond timing capabilities. The Berkeley Advanced Light Source is such a machine.

The committee strongly recommends no action on the lower energy machine interfere with the timely pursuit of the higher energy machine.

The inclusion of support in the fiscal year 1985 budget for the development of insertion devices at existing facilities at Stanford and Brookhaven are certainly in line with our recommendation.

We assume as well that in DOE there is support for the R&D efforts necessary to build the next generation of machines.

[The prepared statements of Dr. Knotek and Dr. Eisenberger follow:]

PLANNING STUDY FOR ADVANCED NATIONAL SYNCHROTRON-RADIATION FACILITIES

SELECTED SECTIONS FROM THE REPORT

The report of a study sponsored by the Department of Energy, Office of Basic Energy Sciences, and cochaired by Peter Eisenberger and Michael L. Knotek.

A new generation of synchrotron-radiation sources based on insertion devices offers gains in photon-beam brilliance as large as the gains that present-day synchrotron sources provided over conventional sources. This revolution in synchrotron capability and its impact on science and technology will be as significant as the original introduction of synchrotron radiation. This report recommends that insertion-device technology be pursued as our highest priority, both through the building of new facilities and through the full development of insertion-device potential on existing machines.

PREFACE

This report presents the results of a study by an ad hoc committee sponsored by the Department of Energy (DOE), Office of Basic Energy Sciences, with the charter to "solicit and evaluate ideas from synchrotron-radiation providers and users as to the future opportunities and technical needs for synchrotron-radiation-based research." The committee was further charged "to establish from the available options a set of priorities for the timely development of both existing and new facilities that can meet those needs."

This study critically evaluates the current status and opportunities for synchrotron radiation (SR)-based science and technology, facilities, and users. The evaluation serves as the basis for a series of recommendations for SR that includes upgrading of existing facilities, new instrumentation, new facilities, and methods of increasing user participation. While the focus of the report is a series of recommended actions, it also contains data, analyses, observations, and criticisms, so that it can serve as a resource for future deliberations.

Judgement Criteria

Our judgements were based generally on the new science and technology offered by the next generation of machines and specifically on the way in which the properties of new sources lead to new experimental capabilities. Our analysis took into account the technological barriers that define the limits of SR sources and various issues affecting the use of these sources by the scientific community.

Methodology

The objective of conducting a comprehensive and critical scientific review influenced the choice of the committee members and the procedures adopted to obtain and evaluate the needed information. The committee membership of seventeen, listed at the end of this preface, included 12 SR users; the members were drawn from universities, industry, and DOE and Department of Defense (DOD) laboratories, and they represent a wide range of disciplines.

To further broaden the representation, we solicited the testimony and active participation of many other scientists, including the personnel of facilities involved in providing SR. The breadth and sophistication of SR-based science and technology required the participation of all these people, and we thank them for their responsiveness and assistance.

Information was first obtained at a meeting held at Sandia National Laboratories, Albuquerque on October 8 and 9, 1983. Approximately 30 speakers and 80 participants gave testimony on science opportunities, facility needs, user needs, and plans for new facilities, including the proposal for the Berkeley Advanced Light Source (ALS), which we were specifically asked to examine. Over 1000 pages of written technical information was provided to the committee, much of which has been distilled and included in this report. The meeting included special sessions for debate and criticism.

As the study proceeded, the committee issued additional calls for letters of opinion from the community and for technical and factual information necessary in our deliberations. Over a hundred such correspondences were received from a broad range of scientific, technical, and institutional interests. Their input has been evaluated, distilled, and, where appropriate, included in this report.

The committee then met in executive session three times over the next three months, at Stanford, MIT, and Exxon, to evaluate the material it had received, to reach its major conclusions concerning the priorities for SR, and to prepare the report. On November 15, 1983 an interim version of the major conclusions and recommendations was submitted to DOE in the form of a letter, which is included as Appendix A.

Committee Member	Institution
H. K. Birnbaum	University of Illinois
W. F. Brinkman	Bell Laboratories
F. C. Brown	University of Illinois
M. H. Cohen	University of California-Berkeley
P. M. Eisenberger	Exxon Research & Development Company
D. E. Eastman	IBM TJ Watson Research Center
C. S. Fadley	University of Hawaii
K. H. Hodgson	Stanford University
M. L. Knotek	Sandia National Laboratories
F. W. Lytle	Boeing Company
D. E. Moncton	Brookhaven National Laboratory
D. J. Nagel	Naval Research Laboratory
J. E. Paterson	Stanford Synchrotron Radiation Laboratory
E. W. Plummer	University of Pennsylvania
J. E. Rowe	University of Florida
H. G. Stever	University Research Associates
P. A. Wolff	Massachusetts Institute of Technology

EXECUTIVE SUMMARY

Introduction

Throughout the development of modern science and technology, electromagnetic radiation has been the most effective of exploratory probes for the discovery of structural characteristics and for the understanding of physical processes. Success in such discoveries has been intimately linked to evolution and revolution in the technology of photon generation. The electric light, the discharge lamp, the x-ray tube, and the laser each ushered in new eras of science. We can now add to this list the most versatile of sources: synchrotrons, or storage rings for the generation of synchrotron radiation (SR).

SR has the unique capability of providing radiation over eight decades of the electromagnetic spectrum, from 10^{-3} to 10^{5} eV. Thus, it reaches from the infrared, the visible, and the ultraviolet, through the soft and hard x-ray domains, and up to the gamma-ray region. Within the last few years we have become confident that SR facilities can be built that will provide unprecedented control of all the important characteristics of a photon beam: source size, spatial coherence, temporal coherence, spectral range, polarization, and time structure. As a source of electromagnetic radiation, only lasers and perhaps plasma sources will maintain any superiority for specific applications.

In the brief history of experimentation in the newly emerging field of SR science and scientific measurements, there are already significant accomplishments in a wide variety of fields. In solid state physics and in surface science, bulk and surface electronic structures have been measured. Grain boundaries and interfaces of important semiconductors and metals have been studied. Surface bond lengths have been determined to a degree of resolution that is important to the study of surface chemistry. In phase-transition physics, the first studies of structural transitions in two-dimensional systems have revealed new phases and new transition mechanisms. In biology, SR has been used to define the active site in important metalloenzymes like nitrogenase, the enzyme responsible for nitrogen fixation in plants. In energy research, the concentration and chemical state of impurities in coal and the structure of bimetallic catalysts have been determined. And in medicine a noninvasive, low-dose angiography technique with the promise of wide applicability as a general medical imaging technique has been developed. Although some of the techniques used in SR science have been used earlier with conventional photon sources, the brightness and tunability of SR has carried experiment and measurement far beyond the capabilities of the past.

Though the thrusts to date have concentrated in the basic sciences, technological applications of SR are beginning to emerge, as evidenced by recent SR studies of catalysis, medical imaging, submicron lithography for the computer industry, defect structures in solids, amorphous materials, alloy-structure determination, phase changes in solids, and applications to biological materials.

The SR field has had a similar impact in the industrialized countries of Europe and Asia. All of these countries expect the industrial and defense applications to grow rapidly in significance, and they all are building their array of SR facilities to handle the work. In some countries--West Germany, France, England, the Soviet Union, and Japan--there are SR facilities comparable to those in the USA, and these countries all have high-priority programs to advance their capabilities.

Opportunities have now been demonstrated for orders-of-magnitude improvement in SR capabilities through the use of special insertion devices called wigglers and undulators and of storage rings with improved characteristics; these innovations make it possible to enhance and optimize the radiation for specific studies. The gains are not only in the intensity of the radiation source but also in its optical qualities, which include extraordinary collimation and small source size, variable polarization, and extremely short pulse lengths. This added control will lead to experiments not previously possible.

One sees expanding horizons of experimentation in basic condensed-matter sciences, in materials science and technology, and in chemistry, biology, and medicine, in addition to increased usage of some of the past techniques with better capabilities. The added flexibility offered by higher-brilliance sources will greatly enhance the sophistication of our physical probes and make possible studies of smaller and more dilute samples and of weaker phenomena. The future offers x-ray holography, various microscopies, studies of low-energy excitations and time-dependent phenomena, the determination of the properties of very small particles, and new frontiers in atomic, molecular, and plasma studies.

To meet the challenges and opportunities in both the scientific-research and the technology applications of SR, facilities will be needed that are dedicated to the utilization of insertion devices and that are readily accessible to the whole spectrum of science, technology, and defense interests. New machines dedicated to the utilization of insertion devices, even if they are developed on the most expeditious schedule, will not have significant impact until the late 1980s or early 1990s. Therefore, our recommendations include the full development of existing insertion-device capability, in parallel with the construction of new facilities specifically designed for the use of these devices.

Recommendations and Conclusions

I. Existing Facilities and Projects

The committee recommends that steps be taken to ensure the timely completion of the commissioning of the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory and the Synchrotron Radiation Center (SRC) at Stoughton, Wisconsin. We are encouraged by the actions at NSLS and SRC since our initial letter to the Department of Energy (DOE). To optimize utilization of existing facilities, we recommend providing operations funding, so that such facilities can provide a maximum of beam time in a "user friendly" mode, and continued research funding, so that it will be possible to take full advantage of the facilities.

To realize the full potential of existing facilities, the committee recommends expeditious completion of currently approved projects to construct insertion-device beamlines: the NSLS Phase II project at Brookhaven Laboratory and the SSRL Enhanced Photon Flux Facility (SEPFF) project at the Stanford Synchrotron Radiation Laboratory (SSRL). The future construction of additional insertion-device-based beamlines at existing facilities is strongly recommended.

II. Major New Facilities

The committee believes that major new programs based on the utilization of insertion devices are of central importance for effective progress in materials-science, physics, biology, and chemistry research over the next decade. The committee is therefore unanimous in its recommendations, which follow in order of priority.

1. The design and construction of a high-energy storage ring capable of providing fundamental undulator radiation in the x-ray region of the spectrum up to 20 keV, with an early 1990s target date for full operation of the facility.

To achieve this objective, appropriate research and development funding should be allocated now.

2. The construction of a second, lower-energy ring capable of providing fundamental undulator radiation in the soft x-ray region of the spectrum up to 2.0 keV. This machine should also provide picosecond (ps) timing capabilities. The Advanced Light Source (ALS) is such a machine.

The committee strongly recommends that no action based on the second-priority recommendation interfere with the timely pursuit of the first-priority recommendation.

III. Alternative-Source Facilities

Free-electron-laser (FEL), ultraviolet (UV)-laser, and laser-heated-plasma sources promise to make important complementary contributions at the low-energy end of the spectrum. To provide a complete full-spectrum capability, these sources should be developed in as timely a fashion as possible by their respective technical communities and funding agencies. However, the committee concluded that in the foreseeable future SR will continue to be the premier source of radiation in the soft x-ray and x-ray regions.

IV. Other Comments and Conclusions

The Need for Two Machines and their Relative Priority--The physics governing the performance of undulators dictates that a machine designed to produce x-ray radiation at energies above 10 keV operate at a different energy level than a machine designed for the optimal production of soft x-ray ultraviolet (XUV) radiation at energies less than 2 keV. Using existing or anticipated technology, fundamental undulator radiation at 10 to 20 keV will require a 5 to 6-GeV machine, while optimized undulator radiation at less than 2 keV will require a machine operating at approximately 1.5 GeV. Factors governing the relative priority of these two machines include:

A. There are no dedicated facilities where x-ray undulators can be developed, whereas some limited opportunities for developing XUV undulators do exist.

B. Although the low-energy ring cannot provide undulator capability in the x-ray region, the high-energy machine can access some of the XUV region, albeit with reduced performance.

Commissioning of New Machines -- The difficulties being experienced in the commissioning of the newly constructed machines arise from overzealous attempts at economy, from some deficiencies in the project-management systems, and from a general lack of big-project experience in the materials-science community. These are not fundamental technical problems and should be rectified in future projects.

Improving Access to Facilities -- The access to SR facilities is currently being restricted by two major factors. The first factor is the difficulty experienced by university-based groups in obtaining the funding necessary for participation. We recommend that beamline funding at future and existing facilities be provided in such a way that university-based groups can participate more readily. This cooperation would significantly broaden both the technical base that could contribute to innovations in instrumentation and the scientific base that could contribute to effective use of the facility. A proposal-based, peer-reviewed approach for the selection of outside participants is strongly recommended.

The second factor is the limitation on the participation of industry, university, and government laboratories that are performing applied research. In deciding which groups can participate in beamline usage, there is currently a bias towards fundamental research. The broadening of program-review committees to include applied interests, together with procedures to ensure more "user friendly" instrumentation and the protection of proprietary and classified interests, would increase the participation of applied-research groups.

Continuing Review -- The rapid developments in SR make it appropriate that a committee similar to ours convene periodically to review current developments in the entire field and to make recommendatins for future actions.

Peter M. Eisenberger

Peter M. Eisenberger is currently Director of the Physical Sciences Laboratory at Exxon Research and Engineering Company, Clinton Township, NJ.

Dr. Eisenberger received his BA in Physics from Princeton University in 1963. He received his PhD in Applied Physics from Harvard University in 1967, after which he continued at Harvard in a post doctoral position from 1967-68.

Following his education, Dr. Eisenberger worked at Bell Laboratories as a professional from 1968-1974, and as a department head from 1974-1981, at which time he joined Exxon Research and Engineering Company in his current position.

Dr. Eisenberger is a Fellow of both the American Physical Society and the American Association for the Advancement of Science. In addition, he is an Adjunct Professor at Stanford University where he is currently involved in research on synchrotron radiation.

Michael L. Knotek

Michael L. Knotek is currently Supervisor at the Surface Science Division at Sandia National Laboratories in Albuquerque, NM.

Dr. Knotek received his BS in Physics from Iowa State University in 1966. He received his MS and PhD in Solid State Physics at the University of California at Riverside in 1972.

From 1970 through 1972, he worked at Michelson Laboratory, China Lake. He moved to Sandia Laboratories in 1973 and has been head of the Surface Science Division since 1979.

Mr. FUQUA. Thank you very much.
Dr. Grunder.

STATEMENT OF DR. HERMANN A. GRUNDER, ASSOCIATE DIRECTOR, ACCELERATOR AND FUSION RESEARCH DIVISION, LAWRENCE BERKELEY LABORATORY, BERKELEY, CALIF., AND DR. GABOR A. SOMORJAI, CENTER FOR ADVANCED MATERIALS, LAWRENCE BERKELEY LABORATORY, BERKELEY, CALIF.

Dr. GRUNDER. Mr. Chairman, members of the subcommittee, we are pleased to be here today to bring you up to date on the activities of Lawrence Berkeley Laboratory and its Center for Advanced Materials. I have a longer statement and attachments which I would like to submit for the record.

I am the Associate Director of the Accelerator and Fusion Research Division, and hence responsible for the Center's laboratory and facilities, as well as for the generic research which hopefully will lead us to the next generation of soft X-ray and VUV machine, as recommended in the Eisenberger-Knotek report.

Dr. Gabor Somorjai, leader of the Center's catalysis program, is also with us. I will present a brief overview of the development of CAM over the past year, and our current activities with respect to the generic R&D on synchrotron radiation. Dr. Somorjai will give you input and report to you on what the development is with respect to industrial participation and what we expect of industry in the future.

The CAM initiative is intended to be responsive to DOE's commitment to direct its laboratories in an effort to get them into a more productive area, particularly with respect to their interaction with industry. The initiative of CAM is one laboratory's attempt to do its part in order to improve the position of American science and industry in the materials science area.

In this context, the mission of CAM can be described as follows. First, CAM will perform high-quality materials research, responding to the long-range needs of high technology industries. Dr. Narath characterized that as the structured research, this "technology-pull," and we entirely agree at LBL with his characterization and try to follow his advice.

Second, CAM will offer educational and training opportunities, in order to bring along the next generation of scientists and engineers specializing in materials-related disciplines in the environment of close contact to industrial needs. I don't need to tell you how important this activity is, and I don't need to tell you because Dr. Narath already mentioned it—the nearly 400 graduate students which LBL has today, and which we hope can be increased to something like 600 graduate students.

With respect to the management of CAM, the project as a whole, the laboratory has welcomed the advice of the panel. Before fiscal year 1984 began, the laboratory had separated the generic research on synchrotron radiation from the CAM laboratory buildings and the CAM materials research program. Laboratory Director David A. Shirley created a new research division for the laboratory, which was appropriately named CAM. The division is headed by Dr. Kenneth Pitzer, a distinguished scientist and proven scientific administrator. We expect to have a permanent director for the CAM division named by early summer. The future of CAM clearly depends on the experience and vision of the person who will fill this position.

We also anticipated the Narath report by the appointment of the CAM Scientific Policy Board, chaired by John Doyle, vice president for research and development of the Hewlett-Packard Co., who also was a member of the Narath panel—he is the chairman of the panel. And he is committed to giving the policy board a strong voice as CAM refines its goals and programs.

The Policy Board is charged by the laboratory to provide guidance on program selection, evaluation, and termination; also on staffing and funding strategies, and on the mechanism for industry participation. Four of the members of CAM are from industry; namely, as I mentioned, John Doyle, vice president for R&D at Hewlett-Packard; Harold Paxton, vice president for research at United States Steel; James McGroddy, director of organization and planning of IBM; J. R. Thomas, president of Chevron Research Corp.; and J. R. Whinnery, U.C. professor of electrical engineering on the Berkeley campus.

In order to continue with CAM in a timely fashion, modern laboratory space and advanced equipment are critical factors in realizing the goals. We have received and appreciated the advice and review of many groups. Congress' continued support for the two buildings in the fiscal year 1985 building budget will be critical if we are to succeed.

Not in the fiscal year 1985 budget is the one component which we believe is an important part of materials research, and which Dr. Knotek has identified in the summary of his testimony. I would like to address briefly if I may do so, Mr. Chairman, I would like to address briefly the ALS and where it stands in our thinking today.

What excites us at LBL is indeed the fact that the Eisenberger-Knotek panel has concurred with our findings 2 years ago that the storage rings based on magnetic insertion devices are indeed a very substantial step forward; and as Dr. Knotek pointed out, are a revolution as big as the introduction of synchrotron radiation itself.

LBL has proceeded on the generic research, in particular on these insertion devices, and it is fair to say that we are the leading laboratory in the Nation when it comes to the R&D and understanding of such devices.

The opportunities have been mentioned, so I will not dwell on them.

We furthermore agree with the panel on the need for two separate rings if we are to exploit the large range of something like a factor of 10 million in spectrum of electromagnetic radiation. We further agree that the hard X-ray machine has intrinsically substantially reduced performance in the soft X-ray regime. This is, of course, the regime we would like to address because it is the kind of science which we understand and which is technologically possible here and now, whereas the beamlines of the hard X-ray need some R&D, as Dr. Knotek pointed out.

We have learned much from our various interactions with the scientific-industrial community over the last year. We expect to learn more.

At this time I would like to let Dr. Somorjai describe to you how the Center for Advanced Materials Division is applying what it had learned in the new program, and where it sees its future.

Dr. SOMORJAI. Thank you, Dr. Grunder.

Mr. Chairman, members of the subcommittee, with all these reviews of CAM, how to do it sometimes gets lost in why to do it in the first place. And I briefly would like to address that, and then I'd like to tell you what we did since October, since the beginning of CAM, and how the various programs are off to a good start.

Well, I'm sure that this committee knows better than most people that the leadership position of American industry in the world markets is eroding, and this is primarily due to the challenge from, most notably, Japan and West Germany, countries that made a national goal to achieve preeminence in high technology areas. By high technology, of course, I mean science-driven technologies, which are exceedingly important. These areas of challenge include computers, televisions, automobiles, pharmaceuticals, and so on.

Now, in the same time, despite all this challenge, American science is in first place. This is clearly indicated by the Nobel Prizes, by virtually all measures, of foreign visitors coming and virtually beseiging our research institutions to learn from us.

Now, what is the reason for the deterioration of our leadership position in technology when our science is preeminent? Mr. Chairman, I believe the reason is that we are not very good at making the connection between science and industry and between the knowledge that we generate and products.

Now, the Japanese in Tsukuba, which is very near Tokyo, 2 hours by train, started 75 government-sponsored institutes pursuing applied research, long-range applied research, in a variety of fields including synchrotron radiation and catalysis. West Germany has a Max Planck Institute complex system performing targeted research in a large number of centers throughout the country. France has the National Center for Scientific Research which encourages high-level researchers at its many laboratories; and, of course, the Soviet Union has a very large number of government research institutes for the same purpose. Now, you might argue the reasons for the inefficiency of some and the efficiency of others, but there is no doubt that Japan and West Germany are clearly very efficient and leading.

Now, this Science Committee has held many hearings on materials policy, scientific, and engineering manpower requirements, industry, the necessity of maintaining half of our research universities and to meet the needs of science education. An underlying theme of your hearings has been the need to make government-industry-university interaction more productive and effective in order to insure the continued economic health of the country.

Well, I believe CAM is one of such efforts, and a most significant one. Necessarily, government-industry-university interaction may be viewed as a three-legged stool. At Berkeley, at LBL, we already have two of these three legs. The government part, represented by LBL, and the university, represented by the Berkeley campus. Both have long histories of excellence and performance second to none.

Now, Berkeley and LBL are uniquely suited to lead this linkup between universities, national laboratories, and industry. We clearly have the scientific talent, and I have to tell you we also have a proven ability to move our students to industry. In the last 20 years I had about 35 or 40 students; two-thirds of them are performing industrial research in a variety of companies.

It seems now that we should make this extra step to build up the third leg and to make a solid connection to industry. And this is what CAM, the Center for Advanced Materials, is all about. The purpose is to try to make our industry highly competitive internationally and in the high-technology marketplace by providing long-range basic research that provides a foundation for that. Now, how are we going to do that? Well, by asking advice from industry and the scientific community and selecting a few research programs that concentrate on technologically important areas that are important to material science. On October 1, 1983, programs in four areas were established: Electronic materials, structural polymers, and polymer composites, catalysis, and instrumentation in surface science. Professor Pimentel mentioned at least two of these four areas, catalysis and instrumentation.

The fifth program, structural high-temperature ceramics, is starting up this month.

Very briefly, the electronic materials program is concentrating on gallium arsenide which is perceived by the community as the next generation of important electronic materials. The structural materials program has two components: polymers and ceramics. The polymers and polymer composites are focusing on predicting microstructures during processing and has tremendous industrial potential and, again, Professor Pimentel was most eloquent in describing some of them.

The ceramics program is focusing on high-temperature ceramics, to understand it well enough to develop novel engines, or ceramic engines.

The surface science and catalysis program has two elements, catalysis and instrumentation. And since I am the group leader, I can perhaps give you a few examples of the importance of this.

We have already a couple of high technology catalysts, which means that science was responsible for developing them. One of them, Mr. Chairman, I am sure you are using, and that is the catalytic converter on your automobile that was developed from the period of 1972 to 1976, and it is primarily responsible for improving the air quality in the Los Angeles Basin; and if you live there—I'm sure we will get comments on that. Clearly, there are others. The other one is the zeolites. Zeolites are aluminosilicates; you may not hear about them, but the Department of Energy actually had the foresight to sponsor a great deal of research in this area. Zeolites are highly porous materials, and if you take syngas, one can convert syngas to jet fuel or gasoline using this new technology. And if we have another energy crisis, I can assure you that as a result of this basic research we are in a much better shape to build a new technology when it's desired, using these new materials.

The CAM catalysis program will be concentrating on developing, by synthesis and characterization, a new generation of zeolites, aluminosilicates. It will be also concentrating on transition metal compounds—carbides, nitrides, silicides, and sulfides—that are to substitute for precious metals—platinum, palladium, these metals that we all use in our catalytic converters but, unfortunately, they all come from South Africa and the Soviet Union.

It seems to me that the program is nice, but how are we going to move it into technology? And that is the key point of the CAM mission. We had workshops with very large industrial participation, and clearly, industry is very enthusiastic about interacting with us. We will have industrial scientists coming to the laboratory in large numbers; and several large industrial companies—DuPont, Standard Oil of California, DOW, Exxon—already indicated willingness and interest to participate with us in a joint research program. We will be moving these industrial scientists to Berkeley. We will ask industrial managers to advise us, and we will move our students to facilitate this interaction. There will be research collaboration, personal exchanges, and of course, common use of facilities.

Our major problem is that we have no place to put these people; these are new programs, and the buildings are absolutely essential for us to get going. We just simply cannot accept these industrial scientists at this point unless we have a place to be able to carry out a joint research program. So I would like to suggest that both buildings, the surface science and catalysis building and the materials laboratory building, are both exceedingly important for us to proceed on this.

It seems to me that this is a new effort to try to address a hole in our science-to-technology transfer effort; that is, to carry out long-range, basic research that will lead to products on a time scale of 10 to 15 years. And this long-range basic research, by and large, is not addressed by most industrial corporations. There are a few who address that, and they do very well indeed: Bell Telephone Laboratories, IBM, DuPont are very scarce examples of these. I suggest, Mr. Chairman, that this is an important program and I hope we'll do well.

[The prepared statements of Dr. Grunder and Dr. Somorjai follows:]

The Center for Advanced Materials
at
Lawrence Berkeley Laboratory

Testimony
to the
Subcommittee on Energy Development and Applications
of the
House Committee on Science and Technology

by
Dr. Hermann Grunder
Associate Director, Accelerator and Fusion Research Division
and
Dr. Gabor Somorjai
Program Leader, Center for Advanced Materials

February 23, 1984

The Center for Advanced Materials at the Lawrence Berkeley Laboratory

One year ago, David A. Shirley, the Director of the Lawrence Berkeley Laboratory testified before this committee about a vision for a new materials research center that would unite a federal laboratory in a partnership with American industry and universities. The goal of the partnership was to boost the international competitiveness of high-technology, energy-related American industries by performing materials-related research responsive to their long-range needs. At the same time, the close collaboration would both promote innovation and accelerate the translation of basic knowledge into new technology. As a most important contribution, the Center would offer education and training to the next generation of scientists and engineers in fields vital to the future health of these industries and our nation as a whole.

In the world markets, the leadership position of American industry, American companies, and American products has eroded. Our leadership is challenged because other countries--notably Japan and West Germany--have made it a national goal to achieve preeminence in many high-technology areas. Computers, televisions, automobiles, and pharmaceuticals are but examples on a long list.

Yet American science is still in first place. Our scientists win the lion's share of Nobel Prizes. Our scientific journals are read the world around. Our laboratories and major research universities rank among the best. They are besieged by foreign visitors and students eager to learn from us. Moreover, our engineering capabilities and technical achievements are nearly unlimited.

What the other countries are doing better is to make the connection between science and industry--between knowledge and products.

The Japanese have established at Tsukuba a government-supported research farm of 75 institutes, each pursuing applied research in a particular field. West Germany has Max Planck Institutes performing targeted research at numerous centers throughout the country. In France, the National Center for Scientific Research encourages high-level researchers at its many laboratories to work together with industry to improve the productivity of their country.

Such teamwork--government working with the private sector--is not as well developed in the United States as elsewhere. But last year the Congress took a major step in this direction by endorsing the Materials Initiative proposed by the Department of Energy. Part of that initiative was the National Center for Advanced Materials.

Now called the Center for Advanced Materials (CAM), the new research center began operating in temporary quarters on October 1, 1983 as a division of Lawrence Berkeley Laboratory. Already 44 scientists and 44 graduate students are active in the programs. Industry interest has been high, and indications are that several Industry Fellows--industrial researchers who participate in CAM programs at their company's expense--will arrive within the next year. At this point, CAM is alive and healthy, but the full realization of its mission is hindered by a lack of dedicated, centralized, modern laboratories.

In this testimony we discuss the many scientific reviews of CAM programs and the Laboratory's response to the many recommendations. We will emphasize the response to the Report of the Ad Hoc Technical Review Panel (A. Narath, chairman), the continuing review of the Advanced Light Source (ALS), a synchrotron-radiation facility proposed as part of the materials center, and the current status and content of CAM's scientific programs. Other significant events in CAM's history are listed on a detailed chronology attached to this testimony.

The Mission of CAM

CAM was proposed over a year ago as one solution to several persisting national problems. American industry has been losing its competitive edge in the international marketplace. Our preeminence is threatened particularly in the manufacture of high-technology products, such as computers, electronic components, televisions, automobiles, laboratory instruments, pharmaceuticals, structural materials, and chemicals. In these industries, the "stopper" problems preventing advances and frustrating new designs or techniques are almost always materials related. To solve these problems requires well-trained scientists and engineers performing long-term basic research--research too risky to show an attractive return on corporate balance sheets in less than five years. Yet the potential payoff of such research in terms of the economic position of American industries and our international balance of trade promises to be enormous.

CAM contributes to the solution of these problems by performing high-quality materials research responsive to the long-range needs of high-technology, energy-related American industries. Primary emphasis is placed on serving the chemicals, electronics, and manufacturing industries that rely on advanced materials to maintain their competitive position. At CAM, large, interdisciplinary research programs focus on materials-related topics of major importance to the targeted American industries. The primary objective of each program is to enhance the knowledge base relevant to the synthesis, processing, characterization, and use of selected advanced materials likely to become useful to these industries. To support the research, the Center maintains state-of-the-art synthesis and processing equipment and modern instrumentation for surface and bulk analysis and characterization of the materials under study. As part of its mission, CAM develops, perfects, and makes available innovative techniques for materials synthesis, processing, and analysis. These techniques might be based on electron microscopy, nuclear magnetic resonance, synchrotron radiation, or other tools and phenomena.

CAM provides educational and training opportunities--unique among DOE national laboratories--to the next generation of scientists and engineers in materials related disciplines vital to the future health of these industries. CAM graduate students and senior fellows participate in the already rich and stimulating interaction between LBL and the Berkeley campus of the University of California. Throughout its existence, Lawrence Berkeley Laboratory has integrated an educational mission into its performance of research for the Department of Energy. At a time when science education is a critical matter for national policy, CAM harnesses one of our nation's strongest centers for scientific education to meet industry's needs for new materials scientists.

As an experiment in collaboration between industry and a federal laboratory, CAM explores novel methods of cooperation and technology transfer. To this end, CAM includes as major participants in its programs visiting scientists from industry and academia along with graduate students, postdoctoral fellows, faculty members, and staff scientists. Critical to the success of the Center is its responsiveness to industry and its selection of appropriate program areas. In this regard, it is apparent from the chronology (Attachment 1) that Lawrence Berkeley Laboratory has solicited and received much advice over the past year from industry and the scientific community. This advice came from numerous workshops, briefings, reviews, and visits. For example, four workshops held last fall to discuss the scientific programs attracted 235 participants, including 115 industrial researchers representing about 70 companies (Attachment 2). Senior research managers from 15 leading American companies attended a workshop in the spring on industry participation in CAM. Over 200 scientists and engineers representing 19 private corporations, 17 universities, 7 national laboratories, and 4 federal agencies participated in the first users workshop for the Advanced Light Source. In addition to workshops, reviews, and briefings, about 100 individuals representing 50 companies have visited CAM, and CAM program leaders have visited over 25 companies to establish contacts, seek advice, and exchange information, ideas, and perspectives.

The Ad Hoc Technical Review Panel and LBL Response

In addition to these self-initiated reviews, Alvin Trivelpiece, Director of the Department of Energy's Office of Energy Research, convened an Ad Hoc Technical Review Panel to evaluate the elements and activities proposed for the Center. The panel was charged to critique and improve the initial LBL planning, so that the best possible features could be incorporated in the facility, and to guide it so that it would pursue the most appropriate activities in a highly effective way.

The panel, chaired by Albert Narath of Sandia National Laboratories, met at LBL in April of last year and it heard from other members of the materials science community later in the spring. The panel transmitted its final report to Dr. Trivelpiece and he forwarded it in late September to the interested congressional committees and to LBL. In October, LBL Director David A. Shirley sent Dr. Trivelpiece LBL's response to the report, praising it and thanking the Panel for its strong endorsement of the CAM concept and for the suggestions to strengthen the Center. Dr. Shirley's letter of response is attached to this testimony (Attachment 3).

Underlying the recommendations of the review panel was a basic assumption that the Advanced Light Source should be decoupled from the materials science program and reviewed separately by a panel qualified to evaluate synchrotron radiation science. In the fall, DOE convened a Study Group on Advanced National Synchrotron Radiation Facilities to do just that. Co-chaired by Peter Eisenberger of Exxon and Michael Knotek of Sandia, this group recently submitted its final report. In addition, the National Academy of Sciences has formed a committee headed by Frederick Seitz of Rockefeller University to consider and prioritize proposed major materials science facilities including synchrotron radiation sources, electron microscopes, and neutron facilities. The Seitz Committee meets next month to hear from the scientific community. In view of these studies, construction of the Advanced Light Source is not requested in the President's FY 1985 Budget. However, we treat some timely issues related to synchrotron radiation facilities later in this testimony.

The Ad Hoc Technical Review Panel made eight major recommendations in its report. As Dr. Shirley noted in his response, CAM had evolved independently so that some of the suggestions were already incorporated in its new form. For example, as originally proposed, the Center included a dozen scientific programs in three laboratories. By September, four programs--representing research areas of major industrial interest where the CAM effort could make a difference--had been selected for initiation. This change anticipated the Panel recommendation that the CAM program emphasize major roles in a few technologically important areas of materials science.

The following paragraphs state the recommendations of the review panel and indicate CAM's response.

(1) Restate the goals and objectives to clarify the intended technology focus and ALS decoupling.

On October 1, 1983, the Center for Advanced Materials was established as a Division of LBL, with Kenneth S. Pitzer as Interim Director. This Division includes only the materials research component of the initiative. The Advanced Light Source, laboratory building construction, and generic light source research remains under the management of the Accelerator and Fusion Research Division. Decoupling of the materials research (CAM) and the ALS is therefore explicit.

Additionally, CAM has adopted a formal statement of its goals and objectives that expresses three major purposes for the research center.

> "CAM performs high-quality materials research responsive to the long-range needs of high-technology, energy related American industries.
>
> "CAM offers educational and training opportunities to the next generation of scientists and engineers specializing in materials-related disciplines vital to the future health of these industries.
>
> "CAM explores novel methods of cooperation and technology transfer between a federal laboratory and industry to accelerate the translation of basic knowledge into new technology."

(2) Appoint a CAM Director who has experience managing directed-research activities and understands the needs of the industrial community.

Kenneth S. Pitzer, a distinguished scientist and proven administrator, became on October 1, 1983 the Interim Director of CAM. A Search Committee formed during the summer nears the end of its national search for a permanent director. Key qualities the committee is looking for include industry experience, materials-research expertise and attainments, managerial skills, and leadership abilities. Fifty applicants have been screened, and a short list of individuals to invite for interviews will be produced soon. The Committee expects to select the Director in April, and to have him on board by July 1, 1984.

(3) Establish a CAM advisory board for policy guidance, with strong industrial representation.

The CAM Scientific Policy Board was named in October and met for the first time earlier this month. John L. Doyle, Vice President for Research and Development of Hewlett-Packard is the chairman. He is joined by James C. McGroddy, Director of Organization Planning for IBM, Harold W. Paxton, Vice President for Research of United States Steel Corporation, John R. Thomas, President of Chevron Research Company, and John R. Whinnery, University Professor at U.C. Berkeley's Department of Electrical Engineering and Computer Sciences. At its first meeting, the Scientific Policy Board was charged by Dr. Shirley to provide guidance on the program selection, evaluation, and termination process, on staffing and funding strategies, and on mechanisms for industry participation. The board members are very supportive of the Center, eager to help insure that it succeeds, and aware of the difficulties in forging productive relationships between industry and institutions like CAM. LBL is committed to giving the Policy Board a strong voice as CAM establishes its first programs.

(4) Develop a CAM program plan which emphasizes major roles in a few technologically important areas of materials science.

As mentioned earlier, CAM has selected with considerable advice from the industrial and scientific community a few research programs that concentrate on technologically important areas of materials science. On October 1, 1983 programs in four areas were initiated: electronic materials, structural polymers and polymer composites, catalysis, and instrumentation for surface science. A fifth program on structural, high-temperature ceramics started up this month. In fact, these programs represent the initial components of major research efforts in three areas: electronic materials, structural materials, and surface science and catalysis.

(5) Establish an organizational structure consistent with CAM program objectives.

CAM program objectives are to perform high-quality, industrially responsive materials research, to educate the next generation of scientists and engineers, and to accelerate the translation of basic knowledge into new technology. CAM's start-up programs serve as the nucleus of the organizational structure pictured in the attached chart (Attachment 4). Each program is performed by an interdisciplinary team that includes internationally recognized scientists along with Industrial Fellows, several graduate students, and postdoctoral fellows. In this organization, program leaders have a primary responsibility to establish and maintain contact with industry, both to insure that their programs are technologically responsive and to make American industry aware of progress. The Industry Participation Office assists the program leaders in this task by encouraging, facilitating, and documenting interactions with industry.

(6) Implement effective mechanisms for industrial involvement.

Part of CAM's mission is to explore novel methods of technology transfer and cooperation with industry. At its first meeting, the Scientific Policy Board was charged with guiding the Center in this matter. At this point four major modes of interaction are in use or envisioned: personnel exchanges, facilities use, research collaboration, and programmatic guidance.

CAM welcomes industrial researchers who participate in programs as Industrial Fellows. CAM also transfers new knowledge to American companies when its personnel serve as consultants.

Specialized facilities and instrumentation at CAM are available for use by industrial and university scientists. This use is coordinated by the Industry Participation Office in consultation with the investigator responsible for the facility or instrument.

Research collaboration in the form of joint research projects and participation in technical workshops is an important mechanism for industry participation. Already 115 industrial scientists have participated in CAM scientific workshops to advise on program areas and emphases. This participation recognizes industry's stake in CAM research, and allows strong contacts to form between CAM researchers and their counterparts in many American companies. Attachment 3 is a list of the companies represented at CAM workshops.

Finally, CAM seeks programmatic advice from industrial scientists and managers. Only these individuals are aware of the current and future "stopper" problems preventing advances and innovation in high-technology products. Strong industry representation on the CAM Scientific Policy Board and industrial participation in CAM workshops and seminars keep CAM responsive to industry needs.

(7) Develop a funding strategy which integrates DOE Basic Energy Sciences funding with support from DOE's programmatic organizations, as well as from industry.

(8) Develop a staffing strategy which is largely independent of future availability of U.C. Berkeley joint faculty appointments.

CAM is in the process of establishing staffing and funding strategies with the advice of the Scientific Policy Board. In terms of staffing, the Divisional Fellowship program is one mechanism being pursued to attract bright young scientists to career positions in CAM. Although no formalized funding strategy is currently in place, the issue of integrating support from diverse sources is now a real one: industry is pledging money to support specific CAM programs.

Research Programs

As illustrated in the attached organization chart (Attachment 4), CAM includes at this time five program components in three program areas: electronic materials, structural materials, and surface science and catalysis. Research in each program targets specific materials-related "stopper" problems identified by industry. Thus, the emphasis of each program will change as the frontiers of knowledge advance and the needs of American industry evolve.

In the Electronic Materials Program, the initial thrust is on advanced, compound semiconductors, specifically gallium arsenide. The research focuses on the major scientific problems to be solved before viable very-large-scale integrated circuits (VLSI) based on gallium arsenide can be developed by industry. Features of gallium arsenide that made it a particularly attractive material for electronic components are its extraordinarily high speed, low power consumption, insensitivity to ionizing radiation, and ability to emit light.

However, gallium arsenide technology does not rest on as firm a scientific foundation now as silicon technology did in the 1960's. Industry has inadequate basic knowledge of the structure and properties of the material and has also experienced serious practical difficulties that impede the widespread use of gallium arsenide in devices. These difficulties include defects in the crystal structure, surface properties and behavior, and brittleness.

In an effort to solve many of these problems, the electronic materials program at CAM focuses on two goals: first, an understanding of the mechanisms of defect formation in bulk crystals of gallium arsenide, and second, elucidation of the structure and electronic properties of interfaces between gallium arsenide and other materials, such as semiconductors, insulators, metals, gases, or vacuum. Concomitant with this research program will be a continuing effort to characterize the bulk and interfacial properties of the gallium arsenide crystals through both existing and newly developed methods. Throughout, strong consideration will be given to possible application of gallium arsenide crystals in novel devices.

The Structural Materials Program has two components concentrating respectively on processing of polymers and polymer composites and on developing advanced ceramics for high temperature use.

The manufacture of articles from synthetic polymers now has a long history, but it is only recently that high-performance polymeric materials have become a reality. Materials are now being synthesized with strength, thermal stability, and chemical resistance sufficient to consider their use in a variety of environments. The properties of objects made from polymeric materials depend not only on the chemical composition of the polymer and the properties of any filler, but also on the entire history of each materials element during processing. There is a pressing need to make progress on the generic problem of predicting microstructure distribution during processing. The specific aspects of this generic problem differ for different types of polymer and polymer composite materials, and for different classes of processes.

CAM's polymer and polymer composites program will focus on the generic problem of predicting microstructure during processing. Initially, studies will be directed to three classes of polymeric materials that currently have considerable industrial potential and interest: liquid crystal polymers, block polymers and short-fiber polymer composites. Research will also be conducted in three processing areas: co-processing, structure control through polymer-solvent-nonsolvent interaction, and molecular weight distribution control through polymerization reaction engineering.

The ceramics program focuses on providing the increased understanding of ceramic processing and high temperature properties necessary for the development of high-temperature, advanced structural ceramics for novel engine applications. To this end, the research includes four related activities: examining the behavior of colloidal suspensions and the structure of powder deposits made from them, studying the evolution of micro-heterogeneities in densifying powder compacts, investigating high temperature mechanical properties of the ceramics, and evaluating high-temperature erosion and wear of ceramic components. Experiments relevant to ceramic component evaluation will be designed in collaboration with interested industries.

The Surface Science and Catalysis Program also has two elements. These projects focus respectively on catalysis and on instrumentation for surface science.

The purpose of CAM's catalysis program is to perform long-range research in catalysis and related areas of surface science and materials chemistry important to the chemical, petroleum, and pharmaceutical industries. The research focuses on synthesis, crystallization, and physical and catalytic properties of metal compound catalysts. Many metal compounds have advantageous catalytic properties, and some may be suitable replacements for precious metal catalysts or may permit controlled molecular engineering.

The CAM catalysis program seeks to understand the relationship between the synthesis and structure of catalysts and between the structure and catalytic properties. With such knowledge, the preparation of catalysts that possess optimal activity and selectivity will be elevated from an empirical art to a rational science.

Initially the program is studying three types of metal compounds: aluminosilicates, transitional metal compounds, and metalloorganic compounds. Aluminosilicates, such as zeolites, are one of the largest classes of commercial catalysts whose uses range from petroleum cracking to water softening. Zeolites' microporous structure make them highly shape-selective catalysts. Carbides, nitrides, silicides, and borides of transition metals are attractive replacements for expensive precious metal catalysts--such as the platinum in automobile catalytic converters--that must be imported. Metalloorganic compounds with catalytic activity may be combined with other metal compounds to offer two catalytic functions at one time. These materials may be applicable in electrochemistry.

The second component of the Surface Science and Catalysis Program develops advanced instrumentation for surface science. Chemical and physical processes at surfaces underlie a great variety of modern technologies, from catalysis to electronics, telecommunications, and computers. Thus the pursuit of these technologies requires knowledge about surfaces at the molecular, atomic, and electronic levels. To gain the necessary knowledge requires instruments capable of probing surfaces at these levels.

A major initial thrust of this program is to develop a scanning tunneling microscope, modeled after the prototype recently pioneered by IBM in Zurich. This device will be used to study surfaces, and, in addition, to complement new projects to measure the vibrational frequencies of atoms and molecules at surfaces and at interfaces, and to study the adsorption of complex organic molecules or polymers on organic or metal surfaces. All of the experiments and research will be coordinated with a theoretical program involving, first, the use of computer calculations to predict the positions of atoms on semiconductor surfaces and interfaces, and to study the electronic and structural properties of transition metal surfaces and interfaces.

CAM Research Laboratories

Two modern laboratory buildings, the Surface Science and Catalysis Laboratory (SSCL) and the Advanced Material Laboratory (AML), have been requested in the President's Budget to house the research activities of the Center for Advanced Materials. These buildings are essential if CAM is to fulfill its objectives. The Surface Science and Catalysis program will occupy the SSCL, and the Electronic and Structural Materials Programs will share the AML.

Currently the five CAM program components are beginning operation in corners of widely scattered laboratory rooms that are shared with ongoing programs not necessarily related to CAM. Any given program might have research tasks being performed in five or more buildings separated by a mile or more. The integrated, interdisciplinary team approach characteristic of CAM can begin in such quarters, but it cannot thrive.

Furthermore, the available laboratories do not have the modern equipment necessary to support a CAM effort that will lead the development of modern materials technology. From the standpoint of the CAM experiment in industry-government collaboration, modern laboratory facilities are critical. The President's FY 1985 Budget includes funds to complete the SSCL and to do the architectural and engineering design work necessary before the AML can be put out for bids. The continued support of Congress in this area will be an important factor in CAM's ability to realize the goals set for it by DOE and LBL, approved by all review groups, and lauded by industry.

The Advanced Light Source

Following the recommendation of the *Ad Hoc* Technical Review Panel, the Advanced Light Source (ALS) was detached on October 1, 1983 from the materials research component of CAM. As noted by the Panel, the ALS is a user facility that will open new scientific opportunities to many disciplines, not just materials science. Subsequently, DOE formed the Study Group for Advanced National Synchrotron Radiation Facilities, to evaluate the Light Source and to prioritize the needs of the growing national community of synchrotron radiation users. Peter Eisenberger of Exxon and Michael Knotek of Sandia National Laboratory cochaired the group.

The Study Group has just submitted its final report to the Department of Energy. The report endorsed magnetic insertion devices as a major technological advance that would revolutionize synchrotron radiation science by providing vastly brighter beams of light. It urged timely commissioning of the two machines currently under construction in Wisconsin and at Brookhaven National Laboratory, and retrofitting existing facilities with insertion devices where possible.

For future science, the Study Group determined that two new machines are needed--a hard x-ray source and a soft x-ray source like the ALS. Optimized for insertion devices, these machines are necessary to provide American scientists with the brilliant beams of synchrotron radiation required by experiments in many fields, including chemistry, biology, medicine, physics, materials science, and others. No single machine can produce high-quality, usable radiation in all the spectral ranges of interest. These ranges include the infrared, extreme ultraviolet, soft x-ray, and hard x-ray regions of the spectrum-- wavelengths varying over a factor of a ten million.

The Study Group placed a higher priority on a hard x-ray light source. The justification is that no dedicated facilities exist where x-ray undulator capacity can be developed, and that the high-energy machine can access the lower energy region. We, of course, agree with the Panel's recommendation that the scientific opportunities in both regimes of the x-ray spectrum are compelling reasons to build both machines. However, we feel that the reasons for establishing a priority between the two machines are not as compelling. For one thing, the technology is at hand to build and operate a soft x-ray machine, and its price tag is only one-third that of the hard x-ray ring (the cost of an accelerator and associated systems increases linearly with the energy).

The Panel is correct that a high-energy ring simultaneously produces hard and soft x-radiation. However, the brilliance of the soft x-rays is only a tenth of what would be available from a lower-energy machine optimized for this spectral region. Furthermore, in order to use the soft x-rays from the high-energy ring, the rest of the spectrum must be discarded or diverted. But today's optical elements cannot handle the heat load imposed by the beam. The solution is to operate the ring at a very low current to decrease the intensity (and brilliance) of the beam. Under such operating conditions, the brilliance delivered to experiments would be reduced to the level projected for currently operating machines. Thus, the extremely exciting science endorsed by the Eisenberger-Knotek Study Group as justification for an insertion-device-based soft x-ray ring that provides extremely short pulses of light, simply could not be performed.

Although the Advanced Light Source has been held up pending review by the scientific community and a consideration of the relative usefulness of different types of research facilities, Lawrence Berkeley Laboratory has been continuing its leadership role in supporting synchrotron radiation research. This past summer, Lawrence Berkeley Laboratory took an important step towards developing optical elements and detectors for the coming generation of intense radiation sources. It established on August 1, 1983 the Berkeley Center for X-Ray Optics under the management of the Accelerator and Fusion Research Division. The Center will provide specialized expertise on XUV (broadly, 10 eV to tens of keV) radiation techniques and their general applications to science and industry, and it will emphasize the emerging technologies required for the efficient transport, dispersion, focusing, and detection of XUV radiation from synchrotron light and other sources of radiation. The Center, which will consist of a core group at LBL and affiliated research associates from the scientific and industrial community throughout the country, will develop new XUV techniques for scientific applications in physics, chemistry, materials science, and the life sciences. It will be closely associated with synchrotron radiation sources, and will also be involved with other emerging sources of XUV radiation. Already the Center has attracted some of the nation's leading scientists in monochromator design, x-ray optics, and x-ray instrumentation to its staff.

Summary

In fiscal year 1984, the Center for Advanced Materials at Lawrence Berkeley Laboratory has begun to pursue its mission to develop materials research programs that are responsive to the long range needs of high-technology, energy-related American industries. In FY 1985, with continued research and construction funding for the Surface Science and Catalysis Laboratory and the Advanced Materials Laboratory, CAM will grow and develop in consultation with industry more specific goals for its programs.

The Committee on Science and Technology has considered the broad national policy issues of materials research, scientific manpower, and science education. In order to solve the problems that this nation faces in these areas, many efforts by many people throughout the country must be undertaken and these efforts must begin in the near future. There is already a strong base of activities at our universities and national laboratories on which we can build; industry is beginning to recognize that these resources must be utilized more fully. There is a mutual recognition that better ways of interacting must be explored. CAM is one effort by one of the Department of Energy's national laboratories to facilitate that necessary interaction. We know that it will not be the only effort, but we are eager to play our part in solving these difficult scientific problems and to contribute to this nation's economic health and future.

Attachment 1

NCAM/CAM Chronology

1979	Chemical and Material Sciences Laboratory authorized for FY 1980 (no appropriation); CAM includes this building as SSCL.
Spring 1982	Design work commences on Advanced Light Source
Spring 1982	Three-page description and a preliminary budget published in Preliminary Data for LBL FY 1983-1988 Institutional Plan.
June 21, 1982	Field Task Proposal/Agreements submitted to the Department of Energy (DOE).
July 7, 1982	DOE Energy Research Advisory Board, Multiprogram Laboratory Panel visit to LBL: presentations highlighted proposed NCAM.
July 26, 1982	Federal Laboratory Review Panel of the White House Scientific Council visit to LBL: briefings included plans for NCAM science and the Advanced Light Source.
September 2, 1982	Institutional Planning Review: NCAM received prominent treatment.
November 15-16, 1982	NCAM Construction Project Review by DOE Office of Management.
November 24, 1982	Final FY 1984 Field Task Proposal/Agreement on Advanced Light Source submitted to DOE.
December 13, 1982	NCAM Project formed within the Accelerator and Fusion Research Division.
January 6, 1983	Advanced Light Source Technical Review.
January 10, 1983	NCAM Scientific Review.
January 11, 1983	Final FY 1984 Field Task Proposal/Agreements on Scientific Programs submitted to DOE.
February 8, 1983	LBL Director, Dr. David A. Shirley, formally presented NCAM to a forum of the Solid State Sciences Committee, NAS.
March 3, 1983	Testimony of LBL Director, Dr. David A. Shirley, before the House Committee on Science and Technology, Subcommittee on Energy Development and Applications.
March 15, 1983	Formation of the NCAM Industry Participation Office.
March 22, 1983	Site visit by DOE Secretary, Donald P. Hodel.

March 23-24, 1983	Site visit and NCAM review by Dr. Richard Kropschot, Director, Office of Basic Energy Sciences, DOE.
March 28, 1983	Presentation of LBL's FY 1985 materials research plans (including NCAM) at DOE.
April 1, 1983	FY 1985 Field Task Proposal/Agreements submitted to DOE.
April 5-7, 1983	Semi-annual NCAM Project Review by DOE Office of Management, headed by Dr. Ed Temple.
April 22-23, 1983	NCAM Ad Hoc Technical and Programmatic Review Panel visit. Dr. Narath of Sandia Laboratory chaired this panel which was convened by Dr. Alvin Trivelpiece to review the proposed scientific program.
May 26, 1983	DOE Validation Review.
May 9-11, 1983	ALS/SSRL Users Workshop.
May 23, 1983	NCAM Industry Participation Workshop.
July 1, 1983	Response to Energy Research Advisory Board Materials Panel questionnaire on major materials research facilities.
July 25-26, 1983	Synchrotron Radiation Vacuum Workshop.
August 1, 1983	Berkeley Center for X-Ray Optics established.
August 31, 1983	Report of Ad Hoc Technical Review Panel conveyed to DOE (Narath Report).
October 1, 1983	CAM Division formed to manage CAM's materials research programs. Responsibility for construction project remains with Accelerator and Fusion Research Division.
October 8-10, 1983	Planning Study for Advanced National Synchrotron Radiation Facilities--information-gathering meeting (P. Eisenberger and M. Knotek, co-chairmen).
October 10-12, 1983	CAM Electronic Materials Workshop.
October 24-25, 1983	CAM Polymers Workshop.
October 24-25, 1983	CAM Metals Workshop.
October 27-28, 1983	CAM Catalysis Workshop.
October 28, 1983	CAM Scientific Policy Board formed.
November 3, 1983	Semi-annual CAM Project Review by DOE Office of Management.
November 14, 1983	Preliminary Report by Planning Study for Advanced National Synchrotron Radiation Facilities.
December 10-12, 1983	Investigation by Surveys and Investigations Office in response to a request by the House Committee on Energy and Water Development.
February 10, 1984	Scientific Policy Board first meeting.
February 15, 1984	Final Report of Planning Study for Advanced National Synchrotron Radiation Facilities conveyed to DOE (Eisenberger-Knotek report).

Attachment 2

American Companies Participating in CAM Workshops

Chemical Companies
- American Cyanamid
- Amoco Chemical Corporation
- Celanese Research Company
- Dow Chemical Company
- E.I. DuPont de Nemours & Co., Inc.
- Monsanto Company
- Raychem Corporation

Computer, Communications, Electronics
- Bell Laboratories
- M/A Com Gallium Arsenide Products
- General Instrument
- Harris Semiconductors
- Hewlett-Packard Laboratories
- Honeywell, Inc.
- IBM Research
- Intel Corporation
- 3-M Corporation
- Motorola Laboratories
- RCA Laboratories
- Texas Instruments
- Xerox Corporation
- Western Electric
- Westinghouse
- Varian Associates

Manufacturing, Transportation, Aerospace
- Boeing Commercial Airplane Company
- Ford Motor Company
- General Motors Research Laboratories
- Hughes Research Laboratories
- Lockheed Missile and Space Co., Inc.
- Rockwell International Corporation

Petroleum Companies
- Atlantic Richfield Corporation
- Chevron Research Company
- Exxon Research & Engineering Co.
- Mobil Research and Development Co.
- Shell Development Company
- Union Oil Company of California

Primary Materials Producers
- Armco Inc.
- Alcoa Aluminum
- Inland Steel
- J&L Steel Corporation
- National Steel Corporation
- Oregon Steel Mills
- Owens-Corning Fiberglass Corporation
- Republic Steel
- Union Carbide Corporation
- U.S. Steel

Miscellaneous/Small Companies
- Advanced Research & Applications
- Airtron
- ARCOR
- Baker Manufacturing Company
- Bend Research, Inc.
- Cambridge Instruments, Inc.
- Catalytica Associates, Inc.
- Crystal Specialties
- Deacon Research
- DeGuigne Tech. Company
- Charles Evans & Associates
- Filtrol Corporation
- GigaBit Logic, Inc.
- Helionckes, Inc.
- Hexcel Corporation
- Maxwell Laboratories
- Michigan Molecular Institute
- P. Q. Corporation
- Physics International
- SAB Partners
- Therma Wave, Inc.
- United Catalysts, Inc.

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Office of the Director
(415) 486-5111 • FTS 451-5111

Attachment 3

24 October 1983

Dr. Alvin Trivelpiece
Director, Office of Energy Research
ER-1, FORSTL
U.S. Department of Energy
Washington, D.C. 20585

Dear Al:

The Ad Hoc Technical Review Panel has produced a frank, perceptive, and constructive review of the National Center for Advanced Materials (NCAM). In response to a recommendation by the Panel and to subsequent guidance from DOE, we are changing the name of the center to Center for Advanced Materials (CAM) and I will refer to it as such in the remainder of this letter.

I appreciate both the Panel's strong endorsement of the CAM concept and its many suggestions and criticisms that indeed will help us to strengthen and improve CAM. LBL is eager to meet the challenge of establishing a new research center that will contribute significantly and in a new way to the U.S. materials science effort while setting a model for productive interactions and collaborations among industry, universities, and national laboratories.

Since it was originally proposed, CAM has been evolving organizationally, managerially, and scientifically. This evolution has been driven in major part by two factors: contacts we have had with industry, the materials science community, DOE, and the review panel; and the necessity--as the Center approached existence--of establishing viable mechanisms and guidelines to ensure that it becomes the center of excellence for industrially responsive materials research we at LBL envisioned at the outset. As I read through the Panel's report, I am pleased that many of the recommendations align closely with our current plans and thinking, and I will discuss these plans more fully below.

I was also pleased that the Panel shares my concern that the development and management of the Advanced Light Source (ALS) and the Center's materials research program not be mutually interfering. Because of this concern, I have taken administrative measures to assure that during construction and operation the two elements remain separate. In the time required to build the ALS, a strong, coherent, "technology-pull" materials program can certainly be developed.

I agree with the Review Panel that the ALS is not exclusively a tool for materials science or for CAM. However, I am reluctant to sever the bonds between the Center's materials research programs and the ALS for several reasons. Both the scientific programs and the CAM model for interactions between industry and national laboratories will benefit greatly from a strong association with the ALS. Industry response to the ALS has been favorable. I expect many collaborations with industry to be initiated around the ALS and to expand to the Center's materials research. Thus, the ALS would promote and facilitate meaningful and productive interactions with industry. Moreover, the materials research, where appropriate, could be conducted on line at the ALS. Use of synchrotron radiation on such a broad scale would very likely boost the productivity of CAM's technologically relevant materials research programs.

LBL is reaching out to the broad community of synchrotron radiation users, both to assay support for the facility and to receive advice on the currently flexible design parameters. As a first step, we held the ALS/SSRL Users Workshop in May to receive recommendations on the appropriate combination of insertion devices and photon beam lines. Dialogue with several workshop participants and other potential users continues as we strive to tailor the design to meet anticipated future research needs.

In establishing a broad base of support for the ALS, we are emphasizing its unique features--high brilliance, low emittance, and short pulses--that were acknowledged by the Review Panel. With these capabilities, the ALS should appeal to researchers in many fields that now use synchrotron light sparingly or not at all. Biology and biomedicine, as the Panel observes, may benefit greatly from the unique features of the ALS. There may also be novel applications of the ALS in atomic physics, chemical kinetics, geology, and other fields.

I am delighted that a planning study group has formed under the leadership of Peter Eisenberger and Mike Knotek to examine the capabilities of existing and proposed synchrotron radiation facilities in light of the growing and evolving scientific applications for synchrotron light. I look forward to the Panel's recommendations and to the exciting research opportunities that will open up when the U.S. builds its first synchrotron radiation source based on insertion devices.

Although the Narath Panel deferred evaluating the ALS, it recommended that LBL increase its involvement in R&D on advanced light sources and on beam line technology. Along these lines, Lawrence Berkeley Laboratory has initiated an R&D effort on x-ray optics. This program will develop the emerging technologies required for efficiently transporting, dispersing, focusing, and detecting x-ray and vacuum-ultraviolet radiation in support of applications in materials science, physics, chemistry, and the life sciences.

Turning now to the materials science component, I would like to share with you some of the progress we have made since the Review Panel visited in April.

As we enter the Center's first year our top priorities are the search for a director and the establishment of initial programs. To locate and evaluate candidates, we have advertised the position nationally and formed a search committee. I expect the committee to identify soon a few top candidates who have the combination of managerial skills, materials-science reputation, and all-important rapport with industry necessary to provide overall scientific and technical leadership for the Center.

In the meantime, I have established an Interim Program Advisory Committee (IPAC) to provide guidance. This committee urged that Dr. Kenneth S. Pitzer be appointed Interim Director of CAM to assure that the new center has an orderly, productive start up and is managed well until the Director comes on board. Effective October 1, CAM has been a Division of the Laboratory with Pitzer serving as its Interim Director.

The IPAC has also selected and recommended four research programs for initiation in FY 1984. The four programs recommended by IPAC focus respectively on catalysis, electronic materials, structural materials, and instrumentation for surface science. To assure a "technology pull" orientation, these programs will be the subjects of open, technical workshops. Three such workshops are being held this October to solicit industry participation and to obtain industry and scientific community advice on the research direction and planned approach.

To assist the Center, the Laboratory, and the Department of Energy in evaluating the results of the workshops, LBL's Office of Planning and Development will undertake an independent, systematic analysis of research ongoing in industry and at other DOE laboratories in the CAM program areas. On the basis of the analysis and the workshop recommendations, programs judged to be duplicative or off target will be redirected or terminated. Other programs to fill identified needs will be proposed for CAM and developed.

Another matter of considerable interest to me has been the appointment of members to CAM's Policy Board. This board, with strong industry representation, will advise me on policy matters and help oversee the development of CAM. I have already contacted several possible Policy Board members, and I expect, with DOE approval, to confirm the Board within a few weeks. The Board should meet for the first time later this fall to consider the most pressing issues facing the new Center. Some of these issues are detailed in the Review Panel's report.

Since the Review Panel's visit we have rethought the organization of CAM, which now centers around the interdisciplinary, focused programs. These programs replace the three laboratories as the major elements of the Center. This new organizational structure answers the Panel's question about the wisdom of separating synthesis programmatically from the other research activities. Now both synthesis and materials-related device development are integrated into each focused program.

Finally, LBL is committed to assuring that its two materials research laboratories--CAM and the Materials and Molecular Research Division (MMRD)--flourish as separate and distinct organizations. As the Review Panel observes, the research modes of these two groups should be different. The new Center's proper role is to perform materials science that is relevant to industry and that requires an organized, interdisciplinary attack on specific research tasks. The MMRD approach, on the other hand, revolves around principal investigators who pursue research topics of their choosing assisted by postdoctoral scientists and graduate students. The coexistence of MMRD and CAM with different perspectives and goals, but similar drive for excellence and well-trained, high caliber-scientific staff, should benefit the vitality of both organizations.

Effective October 1, 1983, CAM is a division of LBL, on a par with MMRD and the other divisions. Top priority for the interim management of the new division will be the development of strategies to staff CAM appropriately for its mission and to promote industry participation in the research programs. In addition to stimulating industry involvement, CAM will also welcome participation from university faculty and students from any campus.

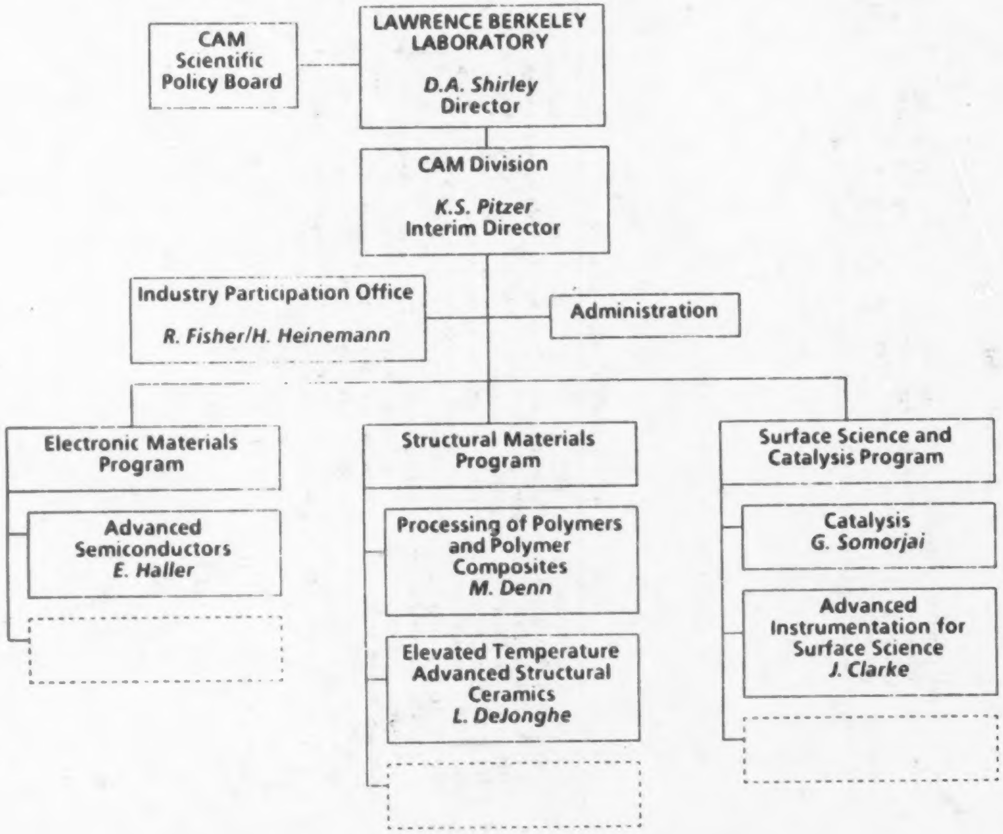
In closing, let me assure you that the Panel Report will be very helpful to us during the Center's formative period. To me, the opportunities before us are very exciting. As a scientist, I am enthusiastic about launching the Center's research activities. As Laboratory Director, I am eager to inaugurate with CAM a new style of collaboration among national laboratories, industry, and universities.

Sincerely yours,

David A. Shirley

cc: A. Narath

Attachment 4: ORGANIZATIONAL STRUCTURE OF THE CENTER FOR ADVANCED MATERIALS


CAM Scientific Policy Board
LAWRENCE BERKELEY LABORATORY
D.A. Shirley
Director
CAM Division
K.S. Pitzer
Interim Director
Industry Participation Office
R. Fisher/H. Heinemann
Administration
Electronic Materials Program
Advanced Semiconductors
E. Haller
Structural Materials Program
Processing of Polymers and Polymer Composites
M. Denn
Elevated Temperature Advanced Structural Ceramics
L. DeJonghe
Surface Science and Catalysis Program
Catalysis
G. Somorjai
Advanced Instrumentation for Surface Science
J. Clarke

Biographical Information

Dr. Hermann Grunder is Associate Director of the Lawrence Berkeley Laboratory and Head of the Accelerator and Fusion Research Division. His research interests include the design of particle accelerators for high energy and nuclear physics research, and for biomedical research. He is also involved in the development of plasma heating techniques, especially neutral beam injectors for fusion energy experiments.

Biographical Information

Professor Gabor Somorjai is Program Leader for the Catalysis Program in the Center for Advanced Materials at Lawrence Berkeley Laboratory and a Professor of Chemistry at the University of California at Berkeley. After receiving his Ph.D. from U.C. Berkeley in 1960, he spent four years working at IBM Research in New York and then joined U.C. Berkeley's Department of Chemistry and Lawrence Berkeley Laboratory's Materials and Molecular Research Division. He is the author of over 300 scientific papers in the fields of surface chemistry, heterogeneous catalysis, and solid state chemistry, as well as two textbooks. Professor Somorjai's principle research interests are in the field of surface science, where he studies the structure of clean solid surfaces, the structure of adsorbed molecules, and catalytic reactions on crystal surfaces. He is a member of the National Academy of Sciences and a Fellow of the American Physical Society and the American Association for the Advancement of Science. Among Professor Somorjai's recent awards are the Colloid and Surface Chemistry Award of the American Chemical Society, the Emmett Award of the American Catalysis Society, and the Kokes Award from Johns Hopkins University.

Mr. **Fuqua**. Thank you very much.

Dr. Narath, the *ad hoc* panel recommended that the construction of the Advanced Materials Synthesis Laboratory and the Advanced Device Concepts Laboratory be deferred until a subsequent review could be made of CAM's program when its program plan is available. What would constitute a tool to be used to judge the acceptability of the plan?

Dr. **Narath**. First of all, let me say that the enthusiastic support on the part of the panel for the CAM activity—it was based on a very specific model, as we all have been discussing here, the idea of a technology pull rather than a science push approach—in the case of the catalysis effort, it seemed to us that based on past accomplishments, the character of the existing staff and others, there was every reason to believe that in that area LBL would achieve success in adopting and pursuing that specific model; and for that reason we recommended strongly that DOE proceed with the Surface Science and Catalysis Laboratory. As far as extending this approach to other activities at LBL is concerned, however, it wasn't clear to us at the time that DOE would necessarily accept our conclusions. For that matter, it wasn't clear whether Berkeley would be able to implement this model in other areas successfully. So we felt that if our support of the venture were used to support further construction at the laboratory, then it only seemed fair that some further review would be carried out of progress and future plans in areas like material synthesis and so on.

Now, the panel did not attempt to reach a consensus as to what would constitute an adequate review. It was clear to us that among the things needed was, first of all, the identification of useful areas for LBL to operate in based on industrial needs and other considerations. The panel simply didn't pursue the question of how DOE should go about arranging for a subsequent review. We were perfectly happy to leave that up to DOE's judgment.

Mr. **Fuqua**. CAM's stated program objectives, if I'm quoting correctly, are to perform high-quality and industrially responsive materials research and to educate the next generation of scientists and engineers, and to accelerate the basic translation of basic knowledge into new technology. Now, could we accomplish that better by funding more basic research for which industry is the performer? What's the advantage of having CAM involved?

Dr. **Narath**. Dr. Trivelpiece this morning referred to the tedious debate as to the relative merits of applied and basic research, and I certainly don't want to delve into that touchy subject. I think it is important to distinguish, however, between two modes of research: One in which the activity is guided by the interests of the individual researcher, on the one hand. On the other hand, research which is motivated to address specific end objectives. I think we all understand that basic science is of fundamental importance; I mean, there's nothing in modern technology that doesn't trace its roots to basic science at some point. On the other hand, to make progress in technology at some point requires translation of basic knowledge into something useful. It's that bridge which determines ultimately the rate at which technology is developed, and several speakers this morning have pointed to the importance of establishing such bridges and addressing technological needs.

In the view of the panel that I chaired, LBL already has some very important ingredients. It already has a large, a very excellent basic science enterprise. And it seemed a worthwhile thing to attempt, to build upon that excellence and to establish new modes of extending basic knowledge, translating it if you will, into technology. Now, how one trades off additional funding for more basic research, nondirected research if you will, versus technology-directed efforts, I can't judge. That's a very difficult matter; it's a judgment call. I think it is true that LBL offers an opportunity to do something that is only possible if you manage to collect a large number of competent people in one place and provide them with adequate facilities and motivation, so I think the opportunity is there and the challenge exists.

Mr. **FUQUA**. Dr. Eisenberger or Dr. Knotek, how vital are the synchrotron light sources to advanced materials R&D in comparison with other research tools, such as neutron sources or high voltage electron microscopes?

Dr. **EISENBERGER**. Our committee did not address that comparison; rather, we looked at the opportunities within the synchrotron radiation field itself. And certainly, as I think you captured in Dr. Knotek's remarks, there is a lot of enthusiasm for the contribution it can make.

Mr. **FUQUA**. Well, did you look at the extent that the synchrotron radiation is an important tool for other fields of science such as chemistry or biology?

Dr. **EISENBERGER**. Oh, definitely. In our report, which is now available for the committee, we addressed the impact of synchrotron radiation across the scientific and technological disciplines. And one of the unique features of it is the breadth of its impact and the diversity of people that you see using it for their very disparate needs.

Mr. **FUQUA**. Dr. Grunder, you or your associate there—is CAM's patent policy in place at the present time?

Dr. **GRUNDER**. We have made great progress on the patent policy. Whether it's in place can only actually be tested in a situation where it occurs and where some progress with industry would be inhibited. We have the promise of the Department of Energy to proceed in such an eventuality with all deliberate speed to address that problem as it might arise; what we can anticipate, we try to do.

Mr. **FUQUA**. Well, how do you plan to handle proprietary information? Is there a policy being developed on that?

Dr. **GRUNDER**. Correct. There is policy being developed on how to handle, in principle, proprietary information.

Mr. **FUQUA**. Mr. Mineta.

Dr. **SOMORJAI**. Mr. Chairman, if I could interject something. We had a workshop, called industry participation workshop which is discussed in some detail—you are absolutely right, one of the key questions of transferring long-range research to industry, and this has been addressed—it has not been solved, but we are making every attempt to try to solve it.

Mr. **FUQUA**. Mr. Mineta.

Mr. **MINETA**. Thank you very much, Mr. Chairman. I apologize for not having been here earlier to hear the testimony of this very distinguished panel, but there are other subcommittees that are meeting this morning, Mr. Chairman.

It looks like we've had an extensive review now, in the past year, of the whole issue about CAM. And now we've gotten to the point where people have said yes, this is a good idea to move forward in the two areas that people have interest in. One is the materials research on long-range industrial problems, and the other about synchrotron sources which, like the ALS, offer broadly exciting scientific opportunities.

Now, I come from an area that is commonly known as Silicon Valley, so that it becomes very important to that region as well as to other areas of this country that are involved in the work product that would come from this kind of effort. Now that we have basically validated these two areas, it seems to me that this other area of the higher energy X-ray sources are also equally exciting; and the question then for us becomes, How do we get from here to there?

We know that the ALS proposal here is going to cost approximately, as I've seen the figures, $72 million. That includes, as I recall—Dr. Grunder, you can maybe help me out on this—the beamline, and what's the other part of it?

Dr. GRUNDER. The $72 million includes the beamlines, the machine itself, and the conventional facilities housing the beamline.

Mr. MINETA. Conventional facilities, right.

Dr. Knotek, I'd like to ask, in your study of this whole issue were you able to address the costs of the high energy machines as well?

Dr. KNOTEK. Well, the high energy machine is in a conceptual design phase at the present moment. We asked Stanford Laboratory, as well as Brookhaven Lab, to look at a rough range of costs that we could expect for the 6 GeV machine. Stanford gave us a number on the order of $170 million, and Brookhaven is not willing to give us a precise number but they say something between that number and $200 million. Now, that would include the synchrotron itself, an injector, and in the case of Stanford it would include 10 beamlines outfitted and ready to operate.

Mr. MINETA. So the numbers range from $170 to $200 million.

Dr. KNOTEK. We can't say those are very hard numbers at this point. We haven't done a complete review by the review panel; it's still in the conceptual design stage.

Mr. MINETA. And what kind of R&D needs to be done to make the high energy machine available?

Dr. KNOTEK. Well, there are a very wide range of R&D topics that could be done. Some of the prime ones are the fact that this high energy machine does produce a lot of power on optical elements, and R&D on the optical elements that are robust enough to handle this sort of power are necessary. As of now, they are a factor of a few to 10 times what is capable of being handled, so R&D in that area has to be done. There is also a great deal of work just on the type of ring parameters they want to have for the big machine. These are very complicated devices. There are several designs being developed, but in order to do it properly you would have to let people work on that long enough to come up with the best design.

There are also a number of topics; one of them, for instance, is whether or not to use electrons in these machines or positrons. Some work needs to be done in that area. There is quite a list of topics, and we have covered some of them in our report.

Mr. MINETA. So you're talking about beamlines, optics, accelerator design. Any timeframe associated with the R&D that would be necessary to get to that high-energy machine?

Dr. KNOTEK. Well, if we look at just how long it would take to get something ready to construction phase, we figure 2 to 3 years.

Mr. MINETA. You mentioned about $170 million. That's as it relates to—what, the research costs, or construction costs?

Dr. KNOTEK. That's the construction costs.

Mr. MINETA. Construction costs. What about the cost of research, then, to get to that point?

Dr. KNOTEK. I don't think we have a hard number on that because we haven't defined the research areas well enough to come out with numbers to request the research funding.

Mr. MINETA. Now, is there a reason why a dedicated high-energy machine is necessary to develop the necessary insertion devices and optics?

Dr. KNOTEK. There is an experiment on the PEP ring at Stanford University, which is much more appropriate for developing an undulator as an engineering test bed for the next generation machine.

Mr. MINETA. And can we use any of those, such as the PEP at Stanford or Cornell, for the research part of this?

Dr. KNOTEK. Well, these two facilities—Cornell is not appropriate for undulator development. The beam properties are not proper for undulator development. Neither of these facilities has any prospect of ever becoming a dedicated facility, so you really could not develop enough capacity to satisfy the need.

Mr. MINETA. You say Cornell definitely, but what about the——

Dr. KNOTEK. PEP—for its foreseeable future, there is no prospect of any dedicated operation on that ring.

Mr. MINETA. Dr. Grunder, when would the ALS be ready for construction?

Dr. GRUNDER. The ALS has had a review in the technical community, and it had preconstruction reviews by the Department of Energy; and indeed, the latest review by the science community was part on the projected budget. So we could proceed with the ALS immediately.

Mr. MINETA. And we heard that there's some R&D needed on beamline before full utilization of the high-energy ring, from Dr. Knotek. To what extent are the insertion devices for the ALS developed already?

Dr. GRUNDER. As I mentioned in my testimony, many of the insertion devices currently in use are built and designed by LBL. For instance, the latest one, the 54-pole wiggler which was shown in Physics Today, is an X-ray line as well as a soft X-ray line, installed. These devices have current state-of-the-art technology which is satisfactory for the uses of the ALS, and therefore we believe the technology is in hand.

Mr. MINETA. What fraction of the ALS construction cost is for beamlines, and to your knowledge should this proportion hold for the high-energy machines as well since Dr. Knotek wasn't sure that he could break it out in terms of the high-energy beamline as a fraction of the cost of the ring?

Dr. GRUNDER. The ALS, if you exclude the conventional facilities, which are roughly $11 million of the $72 million, then the machines and the beamlines are roughly of equal cost; namely, both about $30 million in the case of the ALS. We have not conducted a study with respect to how the beamlines would increase in cost as you go to higher energy; and therefore, I would not want to be in a position to contradict any statements the Eisenberger-Knotek panel had to make. However, if you just look at the simple distances involved, and if you go on that rather crude assumption that the beamline has a certain value per foot, which is a rather crude approximation, you would think that's a ratio of 1 to 1; it's probably holding.

Mr. MINETA. Dr. Somorjai, how far along is the planning for the second building, the AML?

Dr. SOMORJAI. The plans are complete. Clearly, the second building would house the electronic materials program and the structural materials program. It's just awaiting the release of funding to start this construction, I think, a year from now. I believe that the Surface Science and Catalysis Building will be the first one, and then the other building will be the second one. As far as I know, the plans are all complete. The site is chosen, the site studies were done, and environmental impact was completed.

Mr. MINETA. And to what extent does the proposed CAM program require the AML if the advanced light source is not built?

Dr. SOMORJAI. The advanced light source would be an exceedingly important modern tool for materials research. This was clearly shown by Dr. Knotek; but if we don't have that, still, the CAM program—the materials program—includes all the people who would come, industrial scientists, divisional fellows who would be employed, graduate students, and faculty participants. So the needs to run a program do require two buildings; we just simply have no room to put these people. So I think that the personnel needs and the building needs are really independent, in this sense, from the light source; if the light source would be added, perhaps the additional building needs would be taken up by the building areas around the light source.

Mr. MINETA. Thank you very much. Thanks to the panel. Thank you, Mr. Chairman.

Mr. FUQUA. Thank you.

Mr. Bateman.

Mr. BATEMAN. Thank you, Mr. Chairman.

Just one question this morning. As the Department of Energy's programs and activities in materials research and development programs grow, do you feel it's necessary or helpful that there be some continuing advisory panel to point directions and coordinate activities and select areas of emphasis? Anyone on the panel have any reaction to that?

Dr. KNOTEK. Well, in our area in particular, the technology is moving very fast. And for anybody such as you to be well informed and for DOE to be well informed, they need to have something to keep their finger on the pulse of what's happening. There's a lot of money involved in these facilities, there's a long lead time, and proper planning is necessary. So some sort of body to overlook this whole area, the general area of facilities for science, I think is most appropriate.

Mr. **Fuqua**. Any further comments anyone would like to add?

Dr. **Somorjai**. I would like to make a point. I feel, and this is a personal opinion, that we are going through a revolution in our technology. We are moving to high technology, but what we really mean is that science is driving technology; so there is a very strong interrelation between science and the technological and business communities. It's a must.

Now, it's not quite clear how to do this well. CAM is one such effort, but there may be others that will have to be made. It is also clear that we always make the point that basic science is good for technology; but it is also true the other way around. We find very often that technology is a basis, a starting point for new basic research. So there's a coupling in this that I think is going to be the key for this country. Now, some advisory committee or some overview committee that might have representatives from industry, Department of Energy, or other appropriate agencies and other sources might be a very good idea, just to keep an eye on them.

Mr. **Bateman**. But it would appear to this member that where industry chooses to fund its own research and development activities in material sciences, that's pretty much a matter of their own concern if it's their money. Where there is a public-financed involvement and in view of the finite resources, the very, very finite resources from the public purse, it would seem critical to expend that money in the areas that people of the broadest competence indicated should receive the emphasis. Do you feel that some continuing advisory committee or panel then would be a desireable forum? I take it that those who have responded at least agreed generally with that point of view, and that none of you disagree.

Thank you.

Mr. **Fuqua**. Thank you very much for your presentations here this morning. We appreciate your contributions.

Our next panel will be Mr. Robert H. Pry, the vice chairman for Technology of Gould, Inc., and Dr. Frederick Seitz with Rockefeller University.

Dr. Pry, we're very pleased to have you and if you have a statement you wish to submit for the record and summarize it, we'll be pleased to have that.

STATEMENT OF DR. ROBERT H. PRY, CONSULTANT, GOULD, INC., ROLLING MEADOWS, ILL.

Dr. **Pry**. Thank you very much, Mr. Chairman.

One quick correction. In the words of the Navy, I am vice chairman for technology [retired] from Gould. I was vice chairman at the time the report was put together. I'm not retired from the world; I just retired from Gould.

It's a pleasure and an honor for me to be here today to talk about the findings and recommendations of the Energy Research Advisory Board's report on materials research and development. In my written testimony I talk about the role of ERAB; I don't think I have to repeat that here. I think each of you are well aware of the fact——

Mr. FUQUA. We're familiar with it.

Dr. PRY [continuing]. That we are an independent body and we do not speak for the Department or the administration. I will, however, speak for ERAB with respect to this report.

I'd like to have the report put as an amended part of my testimony, if that's possible. It's relatively short so that it shouldn't burden, I think, the Printing Office too much.

Materials research and development throughout history has been a very important part of our technology development and society development. I think that's nowhere more true than in the maze of energy and defense systems.

Recognizing that fact, during his tenure, Deputy Secretary Davis of DOE in November 1982 requested ERAB to undertake a study of materials research and development in DOE. To carry out the work of the study he appointed a materials panel which began its work in January 1983, culminating a report around November of this past year. We were asked to undertake a review that would help the Department insure that its programs are pursuing appropriate research goals and that effective interfaces exist with other agencies and the private sector.

The materials panel formed by ERAB consisted of a dozen leading materials scientists and engineers holding key positions in Government, academia, and industry and represented most of the materials science disciplines. Their names are listed in the report.

In conducting the study, the panel reviewed the relevant work in those Federal agencies with significant materials programs and sought advice from others within the university and industry community. Within DOE the panel reviewed not only the materials programs, but more important, the process of selection of those programs and the process by which the program results were utilized and the organizational framework within which these processes were carried out.

Mr. Chairman, it's my pleasure to state that the Department of Energy headquarters staff, the field operations staff, the management and staff of the laboratories visited, and the other agencies that we talked to were most cooperative and helpful in this study. The single exception was the naval reactors program, whose managers declined to participate. Consequently, I'll make no reference—and there is no reference in the report—on the conduct of their programs, their effectiveness, or their ability to interact with other groups.

It's not really my intent to review all those findings and recommendations; rather, I will concentrate on a few topics relevant to the subcommittee's inquiries today.

First, let me say, as others have said before me in recent years, the Department of Energy Laboratories continue to be troubled by a diffuseness of delegation of authority and responsibility between the DOE central staff, the operations offices, and indeed in several cases between the laboratories themselves. This fuzziness of purpose inevitably leads to a matrix of paperwork and reporting requirements that not only detracts from the time available to do useful work, but also blurs the focus on that person or persons responsible for accomplishing that overall needed result. This problem is particulary acute in the area of materials. The materials researcher and development scientist is often trying to obtain critical knowledge or solve critical problems in specific energy systems. If the research and development authority and responsibility for the specific energy system or subsystem is not clear, it is not clear squared to the materials scientists who is trying to work on problems to solve that systems issue. Ample suggestions already exist in previous reports presented to the Committee on Science and Technology, such as the ERAB report on multiprogram laboratories. I'll not dwell on the matter further here. Suffice it to say, it still needs fixing.

The DOE basic energy sciences program provides a significant fraction of the funding for basic materials research in the United States. The BES materials research program is carried out in DOE multiprogram laboratories, university laboratories, with a minor amount carried out in other institutions. A significant fraction of their materials research funds, about 20 percent in 1983, is spent for the operation and maintenance of unique large facilities situated primarily at the DOE multiprogram laboratories.

The Board concluded that the roles of the BES organization in basic materials research relative to the Nation's overall effort in basic materials research are the following three roles.

First, to provide basic knowledge necessary for the long-term support of DOE energy and defense missions.

Second, to support university research necessary for the education of graduate students who will most likely contribute to the Nation's energy and defense objectives.

And third, to create and operate unique large facilities that support basic materials research and make these facilities available to universities, government, and industrial researchers in materials science.

To insure a planned and measurable balance between these purposes, BES should explicitly provide, in the panel's view, some block funding to support the basic materials research required to make use of these large facilities and to make them most effective. To put it very simply, money is provided for the recognized need of plumbers and electricians for these facilities to keep them operating, but little or no money is provided in the same way to scientists to provide research that might improve upon the facility or its use. Once that needed effort is provided, however, ERAB recommends that all other BES materials programs be competitively funded, after peer review, in DOE laboratories, other agency laboratories, and particularly universities within the guidelines of providing high quality materials science results with long-range relevance to DOE needs, coupling basic materials research to technology development, and training future scientists and engineers. Explicitly calling out these roles in reviewing research programs and proposals, and evaluating the results of those programs, will allow—in our view—BES to obtain a better balance among those roles.

Earlier I remarked that about 20 percent of BES materials research funds are spent on the operation and maintenance of large, unique materials science facilities. This is up from approximately 10 percent 10 years ago through the transfer of existing facilities into DOE from other agencies, and new facilities construction. A review of recent trends and facilities being proposed reveals a likelihood under current procedures that this fraction may well reach 30 percent of the BES materials research funding by 1990.

Such a large fraction of the BES materials science research dollar being spent to operate and maintain large facilities must inevitably be traded off against other DOE roles and priorities, including small but increasingly expensive facilities for new researchers at universities. We have no panacea for solving this problem of balance but to implore DOE to weigh very carefully overall, with the Nation's materials science leaders, each new facility against its other materials science priorities; and in addition, be absolutely sure that outmoded facilities are promptly decommissioned. I think that one of the attributes of most of us in the sciences is that we are packrats; we tend to keep things well beyond their actual years of utility.

I am very pleased to see that this whole matter will be reviewed by the National Academy in a study under the distinguished leadership of Dr. Seitz, who is here with us today.

Having made the above statements about the roles of DOE in basic materials science, let me say a word about materials technology where we believe there is a critical gap which DOE is not adequately filling. In these times of increasing international competitiveness, the United States has continued to excel in the area of basic materials research. But we must remember, in an international free society, basic research results add to the level of the lake of knowledge that the whole world floats in. It is equally accessable to all and we would have it no other way. However, it's only through materials technology developments and materials engineering results applied to our specific system needs that allows us to float higher in the lake of utility than our international friendly competitors. Japan has shown that, I think, very well in recent years. In other words, to allow us to stay ahead.

DOE is doing very well, in our opinion, in BES materials science mission, the basic materials mission. Also, it recognizes the role of materials engineering in supporting already specified systems. DOE falls far short, however, in its emphasis on the generic materials technology development that might allow some of our critically needed but currently uneconomic and impractical energy systems be respecified and become successful with new materials. I don't want to create the impression here that no such work is going on. New approaches to solar to electricity conversion materials and systems, one or two new high temperature corrosion-resistant materials are getting attention in fact. Some increased generic materials technology development work is in place; for example, in the fossil energy systems programs.

I'd like to recall to mind the two examples that we used this morning on high temperature ceramics materials, or what I used to call, in the days when I was working on it, the crockery turbine, and the high temperature ordered alloys, nickel-aluminum ordered alloys that Al Trivelpiece mentioned earlier. Now, those were considered to be breakthroughs in materials science, and indeed they are; however, they are breakthroughs in the same sense as a pure mathemetician says that he has a breakthrough when he proves that a solution to a problem is possible. It takes the applied mathemetician, for example, once that is proven possible, to actually find a general solution. It then takes the mathematically oriented mechanical engineer or hydraulic engineer to then take that solution and make a quiet submarine to go beyond 50 knots. That latter, of course, is the role of the industrialist to make happen.

We heard ample testimony this morning about what is needed to prove that something is possible. The NCAM proposal is still in that area, proving that new materials are possible. The part that is missing is the generation of generic materials that, in fact, can solve specified issues. Let me illustrate with the example of the nickel-aluminum alloy. That traditionally has been extremely brittle material. People know that it will operate and be oxidation-resistant at very high temperatures, but you couldn't roll it, you couldn't form it, and if you put it in an engine and ran through—in the turbine case, they usually use the chicken test, that is, they throw a chicken in the front end to see what happens to it, and what comes out the back end is a combination of chicken and nickel-aluminum alloys. The same thing is true with ceramics.

In order to make that successful, one not only has to know that it will do something besides break when it bends; you also have to go through at least 100 to 1,000 other questions at issue. What happens when eroded at very high temperatures, what happens under conditions where you have the gases of combustion, what happens when you have a slag that goes on it, what kind of long-term diffusion occurs in the material that may degrade it, what happens to very high temperature creep. All of those issues must be solved before you really start to tailor the material for the specific application in a gas turbine or in an engine. That part of the technology, that part of the research in materials is not done, by and large, in DOE; and it is a critical gap that allows other countries to take our results and move forward faster than we do.

Sorry to take the time on that, but many people in ERAB itself did not understand that issue, and we spent many hours at it.

It's those kinds of programs, in our opinion, that does provide that essential glue between materials science knowledge and materials engineering support that generates and promotes real materials solutions to systems problems. Recommendations are made in the report for incorporating more of this work within DOE and keeping it coupled to systems programs and organizationally visible. The problem is, generally speaking, over the years AEC, in the old days, had such programs; but they got eroded. If you put them in basic energy science, it's not neat enough for them; I mean, it's not basic enough. If you put it in the systems program, those tend to go away when there's a budget crunch because the solutions are still a few years off and they have to get on with the system.

Let me bring it home dramatically, if I may. In the early to middle 1950's, a number of people in the materials engineering community were making it as clear as they could to the people who were trying to make nuclear reactors that 304 stainless steel had an Achilles heel, a stress corrosion cracking, and that other materials should be researched and should be developed to fulfill that need. The general opinion was, we can't do that; it would take 15 years. We've got to get on with it. Well, gentlemen, it's still going to take 15 years because we didn't get on with it. I think those generic programs just must be funded within DOE in order to assure that that progress takes place.

Finally, the report does address what steps might be taken to better couple DOE materials activities with industry. Some of these recommendations, I am happy to say, have been made before and, in fact, some are being implemented. And, I might say, with surprisingly good results. I can really only further encourage DOE increasingly to look at itself not as a conservative restraint on technology development, but as a catalyst, a stimulus, and a proactive agent for technological change within the industrial community and the society at large.

This completes my statement. I will be pleased to respond to any questions you may wish to ask.

Mr. Chairman, only one final remark. I was struck by your comment about the husbanding of Government resources and making sure that we do not do the things that industry does. My own view of that issue—indeed, you are correct—but my own view of the issue is that we are both with the Government and with the industry money attempting to accomplish the same purpose, to make our society as technologically advanced and as good for our citizens, from both sides of that: There is no such thing as two sides of that issue, in my view. We must learn how to work together far better in the future.

Thank you very much.

[The prepared statement of Dr. Pry follows:]

TESTIMONY OF ROBERT H. PRY, MEMBER, ENERGY RESEARCH ADVISORY BOARD AND CHAIRMAN, ERAB MATERIALS RESEARCH AND DEVELOPMENT PANEL

Mr. Chairman, it is a pleasure and an honor for me to appear before the Subcommittee on Energy Development and Applications to discuss the findings and recommendations of the Energy Research Admisory Board's (ERAB) report on Materials Research and Development.

ERAB is an independent science and technology committee appointed by the Secretary of Energy to advise the Department of Energy. Operating under the provisions of the Federal Advisory Committee Act, the Board reports to the Secretary and Deputy Secretary. All of its studies are carried out explicitly at their request.

ERAB's role is solely advisory. It reflects the perspectives of a diverse group of private citizens, scientists, lawyers, economists and engineers, who are knowledgeable about energy technologies, but who do not make policy or implement decisions for the Government.

In discussing the Materials Research and Development report with you, I am speaking as the chairman of the Materials Research and Development panel of ERAB and as member of ERAB and not for the Department or the Administration.

The Materials Research and Development report is appended to my formal testimony. In order to better assure that my remarks are taken in proper context, I respectfully ask that this rather short report be included in the record.

Throughout history, but more importantly recently and for the foreseeable future, the development of new products, new systems and new services will depend heavily on the development of new and improved materials and the process of making them. Nowhere is this more true than in the area of energy and defense systems.

Recognizing that fact, Deputy Secretary Davis of DOE in November of 1982 requested ERAB to undertake a study of Materials Research and Development in DOE. To carry out the work of this study ERAB appointed a materials panel which began its work in January of 1983, culminating in a report Materials Research and Development dated November 1983.

In undertaking this study, ERAB was asked to undertake a review that would help the Department insure that its programs are pursuing appropriate research goals and that effective interfaces exist with other agencies and the private sector.

The Materials Panel formed by ERAB consisted of a dozen leading Materials scientists and engineers holding key positions in government, academia and industry and represented most of the materials science disciplines. Their names are listed in the report.

In conducting the study, the panel reviewed the relevant work in those federal agencies with significant materials programs and sought advice from others within the university and industry community. Within DOE the panel reviewed not only the materials programs, but perhaps more important, the process of selection of those programs, the processes by which the program results were utilized and the organizational framework within which these processes are carried out.

Mr. Chairman, it is my pleasure to state that the Department of Energy headquarters staff, the field operations staff, the management and staff of the laboratories visited and the other agencies that provided us with reviews of their materials programs were most cooperative and helpful in this study. The single exception was the Naval Reactors Program, whose managers declined to participate. Consequently no reference is made in the appended report on the conduct of their programs, their effectiveness or their ability to interact with other groups.

It is not my intent to review all of the findings and recommendations in the Materials Research and Development report today. Rather I will concentrate on a few topics relevant to the subcommittee's inquiries.

First let me say, as others have said before me in recent years, the Department of Energy Laboratories continue to be troubled by a diffuseness of delegation of authority and responsibility between the DOE central staff, the operations offices, and indeed even between laboratories. This fuzziness of purpose inevitably leads to a matrix of paperwork and reporting requirements that not only detracts from the time available to do useful work but also blurs the focus on that person or persons responsible for accomplishing an overall needed result. This problem is particularly acute in the area of materials. The materials researcher and development scientist is often trying to obtain critical knowledge or solve critical problems in specific energy systems. If the research and development authority and responsibility for specific energy systems or subsystems is not clear it is doubly unclear to the materials scientist. Ample suggestions already exist in previous reports presented to the committee of Science and Technology, such as the ERAB report on Multiprogram Laboratories. I will not dwell on the matter further here. Suffice it to say, it still needs fixing.

The DOE Basic Energy Sciences Program provides a significant fraction of the funding for basic materials research in the United States. The BES materials research program is carried out in DOE multi-program laboratories, university laboratories, with a minor amount carried out in other institutions. A significant fraction of their materials research funds (about 20% in 1983) is spent for the operation and maintenance of unique large facilities situated primarily at the DOE multi-program laboratories.

The Board concluded that the roles of the BES organization in basic materials research relative to the nations overall effort in basic materials research are the following:

1) To provide basic knowledge necessary for the long term support of the DOE energy and defense missions.

2) To support university research necessary for the education of graduate students who will most likely contribute to national energy and defense objectives.

3) To create and operate unique large facilities that support basic materials research and make these facilities available to universities, government and industrial researchers in materials science.

To ensure a planned and measurable balance between these purposes, BES should explicitly provide some block funding to support the basic materials research required to make the use of these large facilities most effective. To put it simply, money is provided for the recognized need of plumbers and electricians for these facilities but little or no money is provided in the same way for scientists to provide research that might improve upon the facility or its use. Once that needed effort is provided, ERAB recommends that all other, with peer review, BES basic material research programs be competitively funded in DOE laboratories, other agency laboratories and universities within the guidelines of providing high quality materials science results with long range relevance to DOE needs, coupling basic materials research to technology development and training future scientists and engineers. Explicitly calling out these roles in reviewing research proposals and evaluating results will allow BES to obtain a better balance among its roles.

Earlier I remarked that approximately 20% of BES Materials Research funds are spent on the operation and maintenance of large, unique materials science facilities. This is up from approximately 10% ten years ago through transfer of existing facilities into DOE and new facilities construction. A review of recent trends and facilities being proposed reveals a likelihood under current procedures that this fraction may well reach 30% by 1990.

Such a large fraction of the BES materials science research dollar being spent to operate and maintain large facilities must inevitably be traded off against other DOE roles and priorities including small but increasingly expensive facilities for new researchers at universities. We have no panacea for solving this problem of balance but to implore DOE to weigh very carefully with the nation's materials science leaders, each new facility against its other materials science priorities and in addition to be sure that outmoded facilities are promptly decommissioned.

I am very pleased to see that this matter will be reviewed by the National Academy in a study under the distinguished leadership of Dr. Sietz.

Having made the above statements about the roles of DOE in basic materials science let me say a word about materials technology where we believe there is a critical gap which DOE is not adequately filling. In these times of increasing international competitiveness the United States has continued to excel in the area of basic materials research. But we must remember, in an international free society, basic research results add to the level of the lake of knowledge the whole world floats in. It is equally accessable to all and we would have it no other way. However, it is only through materials technology developments and materials engineering results applied to our specific system needs that allow us to float higher in the lake of utility than our international friendly competitors. In other words, allow us to stay ahead.

DOE is doing well in its BES materials science mission. Also, it recognizes the role of materials engineering in supporting already specified systems. DOE falls far short, however, in its emphasis on the generic materials technology development that might allow some of our critically needed but uneconomic and impractical energy systems be respecified and become successful. I do not wish to create the impression that no such work is going on. New approaches to solar to electricity conversion materials and systems, one or two new high temperature corrosion resistant materials are getting attention. Some increased generic materials technology development work is in place in the fossil energy programs, for example.

The facts are, nonetheless, that such programs received major attention in the AEC predecessor organization to DOE but over the years have fallen victim to budget reductions. When placed within BES they are not scientific enough and when placed within the systems programs they usually get cut in bad times because their results are several years away.

These programs however do provide the essential glue between basic materials science knowledge and materials engineering support that generates and promotes new real materials solutions to system problems. Recommendations are made in the report for incorporating more of this work within DOE and keeping it coupled to systems programs and organizationally visible. In addition, of course, such work provides the natural point of involvement with industry, who is ultimately responsible for the commercialization of such new materials.

Finally the report does address what steps might be taken to better couple DOE materials activities with industry. Some of these recommendations have been made before and Mr. Chairman, I am pleased to say some are indeed beginning to be implemented with surprisingly good results. I can only further encourage DOE increasingly to look at itself not as a conservative restraint but as a catalyst, a stimulus and a proactive agent for technological change within the industrial community and the society at large.

This completes my statement. I will be pleased to respond to any question you may wish to ask.

Biography of Robert H. Pry

Dr. Robert H. Pry is currently a management and technical consultant to industry, government and university communities. His major activities include management of strategies for change, technology and government policy, managing the changing relationships between universities and industry, as well as venture management.

Dr. Pry is recently retired Vice Chairrman of Gould Inc., an electronics company, where he was a member of their Executive Management Committee. He had staff responsibility for technical strategy, research and development, external technical relations, corporate manufacturing technology, information and telecommunications technology and information services. He was also Co-chairman of the Management Board for the Gould-Brown Boveri joint venture business in high voltage utility and industrial switchgear.

Dr. Pry joined Gould after serving as Vice President Research and Development for Combustion Engineering Inc. Prior to this position he had a 25 year career with the General Electric Company in research, development and management in materials and electronics science and engineering.

Dr. Pry has published numerous technical publications, book chapters and reports in physics, electronics, metallurgy and materials science, research management, science and technology policy and technology forecasting. He holds a number of patents on materials and devices. He is a Fellow of the American Association for the Advancement of Science and the American Society for Metals. He is also a member of IEEE, APS and a number of other technical societies.

Dr. Pry is a member of the Department of Energy's Energy Research Advisory Board, the Advisory Board of the National Bureau of Standards, the Governing Board of the National Electrical Manufacturers Association, and the Federal Science and Technology Committee of the Industrial Research Institute. He is a member of the Illinois Governor's Commission for Science and Technology and Chairman of the Governor's Task Force on Math/Science Education. He holds board memberships and technical council memberships with several companies and is a member of technical visiting committees at the University of Pennsylvania, University of Illinois and Massachusetts Institute of Technology.

Dr. Pry received his undergraduate education at Texas A&M, Oklahoma University, and the University of Manchester (England), a BS in physics and math at Texas A&I College in 1947 and an MA in 1949 and a PhD in 1951, both in physics, from the Rice University. During World War 11 he served as a cryptographer with the U.S. Army Signal Corp in Europe.

Mr. **Bateman**. Our next panelist is Dr. Seitz, the president emeritus of Rockefeller University, and former President of the National Academy of Science. We're delighted to have you, sir.

STATEMENT OF DR. FREDERICK SEITZ, ROCKEFELLER UNIVERSITY, NEW YORK, NY

Dr. **Seitz**. Thank you very much. Mr. Chairman, it's a privilege to appear before you again.

I'd like to tell you a bit about the role that the National Academy of Science's National Research Council is hoping to play in determining some of the issues related to priorities in connection with materials sciences.

Early in November, the President's Science Advisor, George Keyworth, asked Frank Press, the president of the Academy, for assistance in order to help him in satisfying his own concept of priorities in this area that we've been discussing today. In response, the Commission on Physical Sciences, Mathematics, and Resources organized a committee to work over the next 9 months or so and prepare a report providing informed scientific judgment about needs and priorities for new and upgraded facilities in time for consideration during the 1986 budget.

It is the hope of this committee, which I chair, that we will be able to provide the report to Dr. Keyworth and, of course, to the agencies with which he works, by June.

The facilities to be considered are those with initial costs lying somewhere in the range between $5 and $10 million or more, primarily for research on materials sciences such as pulsed and steady-state neutron sources, vacuum ultraviolet and X-ray synchrotron light sources, and high-voltage electron microscopes.

Because current interest in neutron and synchrotron-radiation sources is so high, primary consideration will be given to these two areas; however, we will not exclude other areas. In fact, our committee will be divided into three panels and one of them will be devoted to other types of possible sources. In addition, our committee has within it individuals who might be called independent benchworkers who do not intend to use very large facilities, so that we have a clear perspective.

As I said, I chair the committee and Dean Eastman of IBM serves as vice chairman; he is one of the vice chairmen of IBM. A balanced group of distinguished scientists has undertaken the task.

In setting the priorities, the committee will consider the following questions, as well as others it deems appropriate.

First, the value and usefulness of each facility for frontier research in materials science and in associated disciplines, such as atomic physics, biology, chemistry, Earth sciences, and medicine. The field of material sciences, of course, cuts across a very broad swath of various fields of science.

Second, availability of other less capital-intensive alternatives for accomplishing comparable objectives.

Third, the quality of scientific leadership and the skilled technical support staff; resources available in other departments at the laboratory or at the university at which it is situated, if it is at or near a university.

Fourth, access to a facility and ease of cooperative use by academic and industrial and governmental scientists. Potential of each facility for training new scientists as well as producing important new research.

Fifth, the leverage or usefulness of a facility for applied research and technology in areas of national priority; for example, economic competitiveness and, of course, security.

The committee will prepare a report setting out priorities primarily for generic kinds of facilities. The committee will, if possible, avoid rating individual laboratory proposals. It hopes to do this in time for fiscal year 1986 budgetary policy decisions. In addressing its task, the committee will review and consider relevant current literature including existing advisory reports, such as those we've had reviewed here this morning; consult with and receive briefings from experts and, if needed, Commission resource papers on particular subjects for committee consideration.

We anticipate that the Department of Energy and the National Science Foundation will provide needed resources for this effort to supplement program initiation funds from the National Research Council.

At its first meeting in late January, the committee formed three subgroups, as I've mentioned: one on neutron scattering—this is chaired by Robert Birgeneau at MIT; a panel on synchrotron-radiation, which will be chaired by Prof. David Lynch of Iowa State University; and a panel on other materials facilities, which will be chaired by Dr. Narath of Sandia Laboratory, who was on the first panel this morning. Those panels will meet in late February and early March, preparatory to a 4-day workshop in mid-March at which the committee will collect and consider information from invited colleagues, including representatives of the interested laboratories and Federal agencies.

Thank you very much.

[The prepared statement of Dr. Seitz follows:]

INVITED STATEMENT BY

Frederick Seitz
Chairman, Major Materials Facilities Committee
to the
House Subcommittee on Energy Development and Applications

Thursday, February 23, 1984
2318 Rayburn House Office Building

MAJOR FACILITIES FOR MATERIALS SCIENCES

Thank you, Mr. Chairman. I am pleased by the opportunity to testify today on the role of the National Research Council in helping set priorities for federal support of major materials research facilities.

My name is Frederick Seitz. I have been a member of the National Academy of Sciences since 1951 and served as its President from 1962 to 1969. Since then I have been at Rockefeller University, serving as President from 1968 to 1978.

Let me outline for you this morning when and how the National Research Council's Major Materials Facility Committee came to be formed as well as its charge, plan of action and current status.

ORIGIN: Early in November, the President's Science Advisor, George Keyworth, asked Frank Press for assistance by the National Research Council in establishing priorities for major facilities in the materials sciences. In response, the Commission on Physical Sciences, Mathematics, and Resources organized a Committee to work over the next nine months or so and prepare a report providing informed scientific judgment about needs and priorities for new and upgraded facilities in time for consideration during the FY 86 budgetary process.

The facilities to be considered are those with initial costs on the order of $5-10 million or more, primarily for research on materials science, such as pulsed and steady-state neutron sources, vacuum ultraviolet and x-ray synchrotron light sources, and high voltage electron microscopes. Because of current high interest in neutron and synchrotron radiation sources, consideration of these will likely predominate but other research opportunities will not be, a priori, excluded. Existing and planned facilities of these kinds are supported by the Department of Energy, the National Science Foundation, and, to a lesser extent, the National Bureau of Standards.

I chair the Committee and Dean Eastman of IBM serves as vice-chairman. A balanced group of distinguished scientists have undertaken the task (roster attached as Appendix 1).

PLAN OF ACTION: In setting priorities, the Committee will consider the following questions as well as others it deems appropriate.

1. Value and usefulness of each facility for frontier research in materials science and disciplines such as atomic physics, biology, chemistry, earth sciences, and medicine.

2. Availability of other less capital intensive alternatives for accomplishing comparable scientific (and educational) goals.

3. Quality of scientific leadership and skilled technical support staff; resources available in other departments at the laboratory or university site.

4. Access to a facility and ease of cooperative use by academic and industrial scientists. Potential of each facility for training new scientists as well as producing important research.

5. Leverage (usefulness) of a facility for applied research and technology in areas of national priority, i.e., economic competitiveness and security.

The Committee will prepare a report setting out priorities primarily for generic kinds of facilities--the Committee will, if possible, avoid rating individual laboratory proposals--in time to benefit fiscal year 1986 budgetary policy decisions. In addressing its task the Committee will review and consider relevant current literature including existing advisory reports, consult with and receive briefings from experts and, if needed, commission resource papers on particular subjects for Committee consideration.

We anticipate that the Department of Energy and the National Science Foundation will provide needed resources for this effort, to supplement Program Initiation Funds from the National Research Council.

CURRENT STATUS

At its first meeting in late January, the Committee formed three subgroups: a panel on neutron scattering, chaired by Robert Birgeneau of MIT; a panel on synchrotron radiation, chaired by David Lynch of Iowa State University; and a panel on "Other" materials facilities, chaired by Albert Narath of Sandia Laboratory. Those panels will meet in late February and early March, preparatory to a four-day workshop in mid-March at which the Committee will collect and consider information from invited colleagues including representatives of the interested laboratories and federal agencies.

We expect to complete at least an interim report by mid-June 1984.

Committee on Major Facilities in Materials Sciences

Frederick Seitz (CHAIRMAN), Rockefeller University
Dean E. Eastman (VICE-CHAIRMAN), IBM T.J. Watson Research Center
Richard B. Bernstein, University of California, Los Angeles
Robert J. Birgeneau, Massachusetts Institute of Technology
Jerome B. Cohen, Northwestern University
Harry G. Drickamer, University of Illinois
Mildred S. Dresselhaus, Massachusetts Institute of Technology
Peter Eisenberger, Exxon Research and Engineering Co., Annandale, NJ
Donald Engelman, Yale University
Peter Jesson, E.I. du Pont de Nemours & Co., Inc.
Walter Kohn, University of California, Santa Barbara
David W. Lynch, Iowa State University
Albert Narath, Sandia Laboratory, Albuquerque, NM
William D. Nix, Stanford University
Ed Rubenstein, Stanford University Medical Center
John J. Rush, National Bureau of Standards
Albert I. Schindler, Naval Research Laboratory
William P. Slichter, Bell Laboratories
Joseph V. Smith, University of Chicago
Richard Stein, University of Massachusetts
H. Guyford Stever, Universities Research Assn., Washington, D.C.
John M. White, University of Texas at Austin

Mr. BATEMAN. Thank you, Doctor.

Dr. Pry, I was intrigued that you commented that your committee or panel had had excellent cooperation from among various agencies save one, and that was from the naval reactor program. Was any reason given for their lack of interest or participation or cooperation?

Dr. PRY. None, sir.

Mr. BATEMAN. Intriguing.

Dr. PRY. I thought so. [General laughter.]

Mr. BATEMAN. Has no one suggested that it was rooted in notions of national security or confidentiality of their——

Dr. PRY. We had no such problem with Sandia or Los Alamos.

Mr. BATEMAN. This is the same——

Dr. PRY. Incidentally, most of the panel members had Q clearance and top secret clearance, so there shouldn't have been a problem. Including myself.

Mr. BATEMAN. For the second year in a row, the Department of Energy is requesting large increases in the materials science areas. Do you believe that these additional funds can be used wisely or do you think we might be moving more rapidly than we are equipped to spend the money well or wisely?

Dr. PRY. No, I don't think that's the case. As I said, I do believe that there is a considerable gap between what is done in the basic materials sciences and where most of U.S. industry picks up. The kinds of work that I talked about, and Al did too, this morning, on nickel-aluminum is still about 10 years away from being in anything. There's just that much time that is required to do all the developmental work on that class of materials, of ordered alloys, to find the ones that, in fact, are going to be the most useful. It's that gap which other countries do emphasize in their government research which we, generally speaking, do not emphasize in our Government research except in the defense areas where the Government, of course, is both the doer and the customer.

Mr. **Bateman**. Both of you gentlemen have significant roles that you have or are playing in advisory capacities and with some review or evaluation process of what's being done. Do you feel that there is a need for something beyond this random, occasional, ad hoc evaluation committees or boards or do we need some continuing, more permanent advisory board or panel?

Dr. **Pry**. Well, I can first answer that. ERAB is, of course, a continuing board for the Department of Energy. Other departments, the National Bureau of Standards, for example—I am on the Legislative Oversight Board for the National Bureau of Standards, as well. Many of the other agencies do use outside civilian support on a continuing basis, so that is in base.

I think that the issue here with respect to materials science is one that I say, in the defense arena, has been in my view satisfactorily solved. We are just new in Government research in the commercial arena, except for the Bureau of Standards. In most other areas it has been recognized over the years that industry does the whole job. We have simply come to both crisis situations that require Government intervention, developments that require such long times; and our international interests require that the Government be there, searching out what their role is in the development phase. That's an issue that we've been struggling with for the last 10 years, as you well know. Through the past two administrations we have been trying to grapple with how to deal with that in-between area where the Government is not the customer, but where its constituents are, in terms of the benefits to society. We are just now, I believe, beginning to recognize that the Government and industry are not adversary parts of the society. In point of fact, each has a complementary role that should support each other. I do believe, that in time, as we search this out and recognize that industry's gain, in many cases, is also society's gain, the Government can supply a supporting role in technology development. I am just simply trying to hasten that day.

Mr. **Bateman**. I should have made it clear in my question that the focus of it was in the materials processes or areas.

Dr. **Pry**. Yes, sir.

Mr. **Bateman**. Dr. Seitz, do you have a comment?

Dr. **Seitz**. In my own experience, the Government agencies do a very good job of making certain that there are advisory committees, either ad hoc or continuing, to take care of what is needed. I think that Mr. Pry's point is a good one; in many ways the transfer from the basic side to usefulness is handled faster in some other countries than it has been in recent years in our own, and it's highly important that we catch up. In the past—say, before World War II and during World War II—we were excellent. It's in the intervening period that for one reason or another, we have slipped.

Mr. **Bateman**. There is no clearly identifiable reason for our lesser performance?

Dr. **Seitz**. No. I think we had it easy for a while, and now times are going to be more competitive.

Mr. **Bateman**. Perhaps we might say that necessity is the mother of invention, and we haven't found the necessity yet but we're finding it?

Dr. **Seitz**. That's right.

Mr. **Bateman**. Well, thank you very much. I'm sure the committee is grateful for your testimony and though many of them are unable to be here this morning, I'm sure that they will have great interest in the record that you've helped us make. Thank you very much.

[Whereupon, at 12:40 p.m., the committee recessed, to reconvene at the call of the Chair.]

APPENDIX I

QUESTIONS AND ANSWERS SUBMITTED FOR THE RECORD

DON FUQUA (Fla.), Chairman

ROBERT A. ROE, N.J.
GEORGE E. BROWN, JR., CALIF.
JAMES H. SCHEUER, N.Y.
RICHARD L. OTTINGER, N.Y.
TOM HARKIN, IOWA
MARILYN LLOYD, TENN.
DOUG WALGREN, PA.
DAN GLICKMAN, KANS.
ALBERT GORE, JR., TENN.
ROBERT A. YOUNG, MO.
HAROLD L. VOLKMER, MO.
BILL NELSON, FLA.
STAN LUNDINE, N.Y.
RALPH M. HALL, TEX.
DAVE MC CURDY, OKLA.
MERVYN M. DYMALLY, CALIF.
PAUL SIMON, ILL.
NORMAN Y. MINETA, CALIF.
RICHARD J. DURBIN, ILL.
MICHAEL A. ANDREWS, TEX.
BUDDY MAC KAY, FLA.
TIM VALENTINE, N.C.
HARRY M. REID, NEV.
ROBERT G. TORRICELLI, N.J.
FREDERICK C. BOUCHER, VA.

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HAROLD P. HANSON
Executive Director
ROBERT C. KETCHAM
General Counsel
DAVID S. JEFFERY
Minority Staff Director

February 28, 1984

Alvin W. Trivelpiece, Director
Office of Energy Research
U.S. Department of Energy
Washington, D.C. 20585

Dear Dr. Trivelpiece:

Thank you for your excellent testimony before the Subcommittee on Energy Development and Applications on February 23, 1984. Attached are some additional questions that Members of the Subcommittee would like you to answer, in order to supplement the record of the hearing on this topic. In addition, a larger set of questions based upon the fiscal year 1985 budget request for Supporting Research and Technical Analysis is enclosed.

I would appreciate your responses to the hearing questions by March 9, 1984, and to the longer set by March 23, 1984. If you have any questions regarding this request, please contact Dr. Harlan Watson of the EDA Subcommittee staff at (202) 225-4320.

Sincerely,

Don Fuqua

DON FUQUA
Chairman

DF:Hcw
attachment

QUESTIONS FOR DR. TRIVELPIECE
FY 1985 DOE AUTHORIZATION FOR SUPPORTING RESEARCH AND TECHNICAL ANALYSIS—SET I

1. **For the period FY 1983 - FY 1985, please provide, by BES subprogram, actual and estimated operating expenses, capital equipment, and construction funding.**

Answer: Please see the table below for the requested information.

BASIC ENERGY SCIENCES

	FY 1983	FY 1984	FY 1985
	(Dollars In Thousands)		
NUCLEAR SCIENCES			
OPERATING EXPENSES	$30644	$37900	$49755
CAPITAL EQUIPMENT	1556	2150	2950
CONSTRUCTION	0	270	300
SUBPROGRAM TOTAL	32200	40320	53005
MATERIALS SCIENCES			
OPERATING EXPENSES	108163	125110	141480
CAPITAL EQUIPMENT	8510	12780	15450
CONSTRUCTION	3000	16440	31720
SUBPROGRAM TOTAL	119673	154330	188650
CHEMICAL SCIENCES			
OPERATING EXPENSES	70000	75500	80930
CAPITAL EQUIPMENT	5510	6520	8840
CONSTRUCTION	400	450	8050
SUBPROGRAM TOTAL	75910	82470	97820
ENGINEERING, MATHEMATICAL & GEOSCENCES			
OPERATING EXPENSES	31050	33670	49045
CAPITAL EQUIPMENT	1920	2120	3000
SUBPROGRAM TOTAL	32970	35790	52045
ADVANCED ENERGY PROJECTS			
OPERATING EXPENSES	8300	9100	10810
CAPITAL EQUIPMENT	290	310	320
SUBPROGRAM TOTAL	8590	9410	11130
BIOLOGICAL ENERGY RESEARCH			
OPERATING EXPENSES	9500	10580	12490
CAPITAL EQUIPMENT	370	400	560
SUBPROGRAM TOTAL	9870	10980	13050
PROGRAM DIRECTION			
OPERATING EXPENSES	3170	3970	3830
SUBPROGRAM TOTAL	3170	3970	3830
BASIC ENERGY SCIENCES	$282383	$337270	$419530

2. For the period FY 1983 - FY 1985, please provide, by BES subprogram, actual and estimated operating expenses, capital equipment, and construction funding going to support facilities.

Answer: For consistency in definition of facilities we are providing information on centers, facilities or groupings of major equipment that have been identified in Question 13. These facilities fall into three categories: 1. User Facilities, 2. Imbedded Facilities -- major equipment or facilities which are part of a research program and are available on a limited basis outside the funded project, and 3. centers that are primarily operated to provide a service to the research community.

Thirteen of the fifteen facility/centers identified below fall into the first category. Two of them, Calutrons and TRU, are in the third category. User facilities are those where facility operating support is provided, or is readily identified separately from support for research utilization by the sponsoring DOE subprogram. In most cases, separate Field Task Proposals are submitted by the host laboratory to DOE for facility support. The facilities are:

		FY 1983 ($K)	FY 1984 ($K)	FY 1985 ($K)
ANL: High Voltage Electron Microscope Tandem Facility				
Operating	MS	1065	1185	1350
Equipment	MS	235	900	925
Construction	GPP	0	200	800
Intense Pulsed Neutron Source				
Operating	MS	6095	7012	7466
Equipment	MS	300*	275*	450*
Construction	GPP	70*	25*	145*
BNL: High Flux Beam Reactor				
Operating	MS	8955	9933	12000
	CS	410	420	455
Equipment	MS	200	400	700
	CS	50	60	60
Construction	GPP	66	80	120
	Other	285	0	0
	MS	0	40	500
National Synchrotron Light Source				
Operating	MS	7776	9762	11500
	CS	5370	6350	7630
Equipment	MS	900	800	800
	CS	770	790	340
Construction	MS	100	3100	11100
	GPP	611*	475*	700*
	Other	0	0	100*
LBL: National Center for Electron Microscopy				
Operating	MS	1380	1750	2200
Equipment	MS	300	350	400
Construction		463*	270*	100*

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		FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
LANL: Spallation Neutron Research/Proton Storage Ring				
Operating	MS	1530	1570	2300
Equipment	MS	250	300	600
Construction	GPP	400	0	0
	MS	2700	0	0
ORNL: High Flux Isotope Reactor				
Operating	NS	5590	6150	9270
	MS	1868*	2190*	2370*
Equipment	NS	70	120	80
	MS	200	400	600
Construction	NS	0	0	300
	GPP	0	0	250*
National Center for Small Angle Scattering Research				
Operating	MS	90*	90*	100*
(This is an NSF facility dependent on neutrons from HFIR.)				
Oak Ridge Electron Linear Accelerator				
Operating	NS	3027	3245	3580
Equipment	NS	165	180	500
Construction	GPP	580*	0	0
Shared Research Equipment Program				
Operating	MS	260	290	320
Equipment	MS	75*	290*	325*
Surface Modification and Characterization Laboratory				
Operating	MS	1235	1450	1935
Equipment	MS	257*	595*	825*
Construction	GPP	235*	650*	500*
Transuranium Processing Plant				
Operating	NS	4900	5136	5490
Equipment	NS	100	60	70
Electromagnetic Isotope Preparations Facility				
Operating	NS	820	680	1700
Equipment	NS	200	500	500
SNL-L: Combustion Research Facility				
Operating	CS	5010	5510	6020
Equipment	CS	900	800	700
Construction	GPP	0	100	530

		FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Stanford Synchrotron Radiation Laboratory				
Operating	NS	5894	6790	7980
Equipment	NS	456	490	600
Construction	GPP	0	0	100

* Data provided by laboratories and based on their information or estimates

Eight of the facility/centers fall into the second category of "Imbedded Facilities." They involve specialized pieces of equipment which are central to, and part of, the conduct of a large research project. Their operating costs are usually not separately broken out but are included in the funds provided for the implementation of the research project employing them. The equipment/facility may be made available to qualified users on a case-by-case basis at no cost, when appropriate. The imbedded facility/centers are:

ANL Atomic Spectroscopy Facility
ANL 4.5-MV Dynamitron Accelerator
ANL Pulse Radiolysis Facility
Kansas State University James R. Macdonald Laboratory
Notre Dame Radiation Laboratory Pulse Radiolysis Facility
Notre Dame Radiation Laboratory Radiolysis ESR Facility
ORNL EN-Tandem Facility
Research Computer Facilities

The ANL 4.5 MV Dynamitron and the ANL Pulse Radiolysis Facilities are jointly funded by BES and HENP. Accelerator and Reactor Improvement and Modification funds have been provided to these facilities as follows ($K):

	FY 1983	FY 1984	FY 1985
ANL 4.5 MV Dynamitron (Nuc. Physics)	300	100	150
ORNL EN-Tandem Facility	100	100	0

The Kansas State University James R. Macdonald Laboratory is a university-owned atomic physics facility. Research support provided by BES includes funding for operation of an accelerator. Included in the BES FY 1985 request are funds, $2 million, to initiate upgrading of the accelerator at a total estimated cost of $3.4 million to DOE ($1.4 million will be requested to complete the project in FY 1986). Additionally, the State of Kansas will provide $0.6 million to upgrade the housing for the accelerator.

There are 11 Research Computer Facilities, 10 at DOE laboratories and 1 at a university, each consisting of one or more minicomputers dedicated primarily to a specific thrust of the Applied Mathematical Sciences subprogram of BES. Operation of the facilities is supported within the framework of each of the individual projects. Capital equipment funding for these facilities was $800,000 in FY 1983, $970,000 in FY 1984, and the FY 1985 request is for $1.5 million.

There are three facility/centers besides the Transuranium Processing Plant and the Calutrons in the third category. Service facilities generally do not have a research component directly at the facility except to improve the service provided, and normally operate on a cost reimbursable basis. These three are discussed below:

Ames Laboratory Materials Preparation Center
ANL Premium Coal Sample Bank
LANL Equation of State Library

Ames Laboratory Materials Preparation Center

$K

	FY 1983	FY 1984	FY 1985
Operations - Total	892	950	1076
Ames Laboratory Orders	687	740	826
Non Ames Laboratory Orders	205	210	250

The facility operates on a cost reimbursable basis and has no independent facility operating budget. The center consists of special sample preparation apparatus and personnel trained in its use. Samples which are not available from other sources are prepared on order according to specifications on a best effort basis. The center also provides analytical services and acts as a clearing house/referral system for information about the availability of special research samples.

ANL Premium Coal Sample Program

$K

	FY 1983	FY 1984	FY 1985
Operating	454	645	622

The ANL Premium Coal Sample Program collects, prepares and distributes reference grade samples of a small number of representative coals for the use of qualified researchers to establish benchmark experimental measurements in coal science. Exceptionally uniform samples are specially prepared and stored in an inert atmosphere to ensure the chemical stability of the coal over a long period of time.

Los Alamos Equation of State Library

$K

	FY 1983	FY 1984	FY 1985
Operating total	320	350	250
Operating BES - Materials Sciences	120	125	0
Other - Defense Programs	200	225	250

This facility is a computer based Library of Equation of State data and FORTRAN subroutines developed at Los Alamos which are made available without charge to qualified scientists and engineers.

3. **For the period FY 1983 - FY 1985, please provide, by BES subprogram and by DOE laboratory, actual and estimated BES funding going to DOE laboratories.**

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES

	FY 1983	FY 1984	FY 1985
	(Dollars in Thousands)		
NUCLEAR SCIENCES			
LABORATORIES			
OPERATING EXPENSES			
ARGONNE NATIONAL LAB	$ 1237	$ 1300	$ 1820
BROOKHAVEN NATIONAL LAB	1910	2057	2800
IDAHO NATIONAL ENGINEERING LAB	290	300	520
LAWRENCE BERKELEY LAB	1504	5135	6115
LAWRENCE LIVERMORE NATIONAL LAB	265	210	220
LOS ALAMOS NATIONAL LAB	1288	2300	3075
MOUND LABORATORY	157	140	232
OAK RIDGE NATIONAL LAB	15695	16671	21610
PACIFIC NORTHWEST LABS	244	250	260
STANFORD UNIVERSITY-SLAC	0	50	50
OPERATING EXPENSES	22590	28413	36702
CAPITAL EQUIPMENT			
ARGONNE NATIONAL LABORAORY	100	100	100
BROOKHAVEN NATIONAL LAB	40	50	50
IDAHO NATIONAL ENGINEERING LAB	25	25	25
LAWRENCE BERKELEY LAB	90	265	590
LOS ALAMOS NATIONAL LAB	140	145	225
OAK RIDGE NATIONAL LAB	645	950	1240
PACIFIC NORTHWEST LABS	20	20	20
CAPITAL EQUIPMENT	1060	1555	2250
CONSTRUCTION			
OAK RIDGE NATIONAL LAB	0	270	300
CONSTRUCTION	0	270	300
SUBTOTAL	23650	30238	39252

MATERIALS SCIENCES	FY 1983	FY 1984	FY 1985
	(Dollars In Thousands)		
LABORATORIES			
OPERATING EXPENSES			
AMES LAB	7160	7520	7900
ARGONNE NATIONAL LAB	19990	21000	22260
BROOKHAVEN NATIONAL LAB	20730	23370	27600
IDAHO NATIONAL ENGINEERING LAB	400	550	580
LAWRENCE BERKELEY LAB	7800	13300	15300
LAWRENCE LIVERMORE NATIONAL LAB	1584	1520	1770
LOS ALAMOS NATIONAL LAB	3727	3900	4500
OAK RIDGE NATIONAL LAB	19038	21030	23200
PACIFIC NORTHWEST LABS	1960	2050	2070
SANDIA-CORP	2360	3120	3400
SANDIA, LIVERMORE LABORATORY	910	980	1050
SERI	350	420	450
OPERATING EXPENSES	86009	98760	110080
CAPITAL EQUIPMENT			
AMES LAB	810	750	800
ARGONNE NATIONAL LAB	1670	2220	2700
BROOKHAVEN NATIONAL LAB	1900	1240	1800
IDAHO NATIONAL ENGINEERING LAB	40	170	60
LAWRENCE BERKELEY LAB	790	2670	2200
LAWRENCE LIVERMORE NATIONAL LAB	100	150	200
LOS ALAMOS NATIONAL LAB	600	900	800
OAK RIDGE NATIONAL LAB	2090	2700	2900
PACIFIC NORTHWEST LABS	180	200	250
SANDIA CORP	200	290	340
SANDIA, LIVERMORE LABORATORY	100	140	150
SERI	30	50	100
CAPITAL EQUIPMENT	8510	11480	12300
CONSTRUCTION			
AMES LAB	275	275	600
BROOKHAVEN NATIONAL LAB	0	3140	11100
LAWRENCE BERKELEY LAB	0	2060	12290
LOS ALAMOS NATIONAL LAB	2700	0	0
CONSTRUCTION	2975	5475	23990
SUBTOTAL	97494	115715	146370

CHEMICAL SCIENCES	FY 1983	FY 1984	FY 1985
	(Dollars In Thousands)		
LABORATORIES			
OPERATING EXPENSES			
AMES LAB	2812	2946	3130
ARGONNE NATIONAL LAB	10612	11347	11766
BARTLESVILLE ENERGY TECHNOLOGY CENTER	149	177	186
BROOKHAVEN NATIONAL LAB	12555	13767	14989
IDAHO NATIONAL ENGINEERING LAB	165	120	126
LAWRENCE BERKELEY LAB	6299	6214	6125
LAWRENCE LIVERMORE NATIONAL LAB	235	30	45
LOS ALAMOS NATIONAL LAB	715	719	504
MOUND LABORATORY	978	950	730
OAK RIDGE NATIONAL LAB	7725	7716	7931
PACIFIC NORTHWEST LABS	1300	1310	1414
PITTSBURGH ENERGY TECHNOLOGY CENTER	78	93	87
SANDIA CORP	410	655	533
SANDIA, LIVERMORE LABORATORY	5010	5509	6000
SERI	600	731	839
OPERATING EXPENSES	49643	52284	54405
CAPITAL EQUIPMENT			
AMES LAB	335	447	450
ARGONNE NATIONAL LAB	885	1105	3475
BARTLESVILLE ENERGY TECHNOLOGY CENTER	20	15	22
BROOKHAVEN NATIONAL LAB	1376	1491	1303
IDAHO NATIONAL ENGINEERING LAB	12	11	15
LAWRENCE BERKELEY LAB	918	1071	731
LAWRENCE LIVERMORE NATIONAL LAB	13	3	5
LOS ALAMOS NATIONAL LAB	52	64	60
MOUND LABORATORY	71	71	81
OAK RIDGE NATIONAL LAB	562	691	846
PACIFIC NORTHWEST LABS	90	116	169
PITTSBURGH ENERGY TECHNOLOGY CENTER	5	7	10
SANDIA CORP	29	58	64
SANDIA, LIVERMORE LABORATORY	905	800	700
SERI	44	65	100
CAPITAL EQUIPMENT	5317	6015	8031
CONSTRUCTION			
ARGONNE NATIONAL LAB	300	100	5200
BROOKHAVEN NATIONAL LAB	75	0	600
OAK RIDGE NATIONAL LAB	0	250	200
SANDIA, LIVERMORE LABORATORY	0	100	0
CONSTRUCTION	375	450	6000
SUBTOTAL	55335	58749	68436

ENGINEERING, MATHEMATICAL & GEOSCIENCES	FY 1983	FY 1984	FY 1985
	(Dollars In Thousands)		
LABORATORIES			
OPERATING EXPENSES			
AMES LAB	500	600	725
ARGONNE NATIONAL LAB	2430	2680	3213
BROOKHAVEN NATIONAL LAB	600	630	675
IDAHO NATIONAL ENGINEERING LAB	200	275	295
LAWRENCE BERKELEY LAB	3185	3059	3181
LAWRENCE LIVERMORE NATIONAL LAB	2280	2700	2668
LOS ALAMOS NATIONAL LAB	2789	3590	2950
OAK RIDGE NATIONAL LAB	1380	1690	1856
PACIFIC NORTHWEST LABS	1153	1205	1089
SANDIA CORP	1982	2260	2352
SANDIA, LIVERMORE LABORATORY	550	595	645
OPERATING EXPENSES	17049	19284	19649
CAPITAL EQUIPMENT			
AMES LAB	50	95	20
ARGONNE NATIONAL LAB	190	180	30
IDAHO NATIONAL ENGINEERING LAB	40	20	20
LAWRENCE BERKELEY LAB	610	280	120
LAWRENCE LIVERMORE NATIONAL LAB	200	180	120
LOS ALAMOS NATIONAL LAB	180	170	150
OAK RIDGE NATIONAL LAB	135	190	290
PACIFIC NORTHWEST LABS	55	110	70
SANDIA CORP	100	120	130
CAPITAL EQUIPMENT	1560	1345	950
SUBTOTAL	18609	20629	20599
ADVANCED ENERGY PROJECTS			
LABORATORIES			
OPERATING EXPENSES			
ARGONNE NATIONAL LAB	512	600	700
BROOKHAVEN NATIONAL LAB	30	662	520
FERMILAB	- 8	0	0
IDAHO NATIONAL ENGINEERING LAB	694	240	600
LAWRENCE BERKELEY LAB	400	500	700
LAWRENCE LIVERMORE NATIONAL LAB	204	150	460
LOS ALAMOS NATIONAL LAB	1168	819	900
PRINCETON PLASMA PHYSICS LAB	305	110	300
SANDIA CORP	110	201	200
SERI	143	18	300
OPERATING EXPENSES	3558	3300	4680

CAPITAL EQUIPMENT	FY 1983	FY 1984	FY 1985
	(Dollars in Thousands)		
BROOKHAVEN NATIONAL LAB	106	138	100
LAWRENCE BERKELEY LAB	10	0	0
LAWRENCE LIVERMORE NATIONAL LAB	30	50	100
LOS ALAMOS NATIONAL LAB	94	50	100
PRINCETON PLASMA PHYSICS LAB	20	0	20
SANDIA CORP	30	10	0
CAPITAL EQUIPMENT	290	248	320
SUBTOTAL	3848	3548	5000

BIOLOGICAL ENERGY RESEARCH

LABORATORIES

OPERATING EXPENSES			
BROOKHAVEN NATIONAL LAB	915	980	1200
LAWRENCE BERKELEY LAB	910	1011	1200
LAWRENCE LIVERMORE NATIONAL LAB	20	0	0
LOS ALAMOS NATIONAL LAB	0	0	200
OAK RIDGE NATIONAL LAB	200	200	200
SERI	105	105	120
OPERATING EXPENSES	2150	2296	2920
CAPITAL EXPENSES			
BROOKHAVEN NATIONAL LAB	70	50	50
LAWRENCE BERKELEY LAB	50	50	50
CAPITAL EQUIPMENT	120	100	100
SUBTOTAL	2270	2396	3020

4. For the period FY 1983 - FY 1985, please provide, by BES subprogram and by university, actual and estimated BES funding going to university researchers.

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES

NUCLEAR SCIENCES	FY 1983	FY 1984	FY 1985
	(Dollars in Thousands)		
OPERATING EXPENSES			
COLORADO SCHOOL MINES	$ 47	$ 75	$ 60
DENISON UNIVERSITY	49	49	40
FLORIDA STATE UNIVERSITY	89	96	102
LOWELL, UNIV OF	120	124	130
MICHIGAN, UNIVERSITY OF	158	170	180
MIDDLE TENNESSEE STATE	0	36	40
NEW MEXICO, UNIVERSITY OF	180	129	138
NEW YORK STATE, UNIVERSITY OF ALBANY	41	0	0
NORTH CAROLINA STATE UNIVERSITY	80	50	55
OHIO UNIVERSITY	215	235	250
OREGON STATE UNIVERSITY	30	0	0
PENNSYLVANIA, UNIVERSITY OF	96	92	95
STANFORD UNIVERSITY-SSRL	5894	6736	7880
TENNESSEE, UNIVERSITY OF	224	235	268
OPERATING EXPENSES	7223	8027	9238

	FY 1983	FY 1984	FY 1985
	(Dollars In Thousands)		
CAPITAL EQUIPMENT			
STANFORD UNIVERSITY-SSRL	456	490	600
CAPITAL EQUIPMENT	456	490	600
SUBTOTAL	7679	8517	9838
MATERIALS SCIENCES			
OPERATING EXPENSES			
ARIZONA STATE UNIVERSITY	182	200	232
ARIZONA, UNIVERSITY OF	72	75	82
BOSTON UNIVERSITY	162	0	0
BRANDEIS UNIVERSITY	44	0	45
BROWN UNIVERSITY	362	305	429
CALIF, UNIVERSITY OF, DAVIS	237	223	210
CALIF, UNIVERSITY OF, IRVINE	222	214	268
CALIF, UNIVERSITY OF, LOS ANGELES	61	0	0
CALIF, UNIVERSITY OF, SAN DIEGO	399	438	465
CALIF, UNIVERSITY OF, SANTA BARBARA	244	99	207
CALIFORNIA INSTITUTE OF TECHNOLOGY	302	363	387
CARNEGIE MELLON UNIVERSITY	148	75	120
CASE WESTERN RESERVE UNIVERSITY	201	0	178
CHICAGO, UNIVERSITY OF	138	140	157
CLARK COLLEGE	70	0	85
COLORADO RESEARCH INSTITUTE	0	67	71
COLORADO SCHOOL MINES	152	156	185
COLORADO, UNIVERSITY OF	187	110	120
COLUMBIA UNIVERSITY	79	87	110
CONNECTICUT, UNIVERSITY OF	266	150	151
CORNELL UNIVERSITY	761	1039	805
DARTMOUTH COLLEGE	88	97	125
DELAWARE, UNIVERSITY OF	60	73	80
DENVER, UNIVERSITY OF	153	152	160
EMORY UNIVERSITY	44	0	0
FLORIDA STATE UNIVERSITY	102	0	0
FLORIDA, UNIVERSITY OF	266	105	573
FRANKLIN INSTITUTE	24	25	27
GEORGIA INSTITUTE OF TECHNOLOGY	149	159	172
HARVARD UNIVERSITY	373	120	345
ILLINOIS INSTITUTE OF TECHNOLOGY	- 2	0	0
ILLINOIS, UNIVERSITY OF	3038	3222	3535
KENTUCKY, UNIVERSITY OF	189	264	301
LEHIGH UNIVERSITY	314	76	397
LOUISIANA STATE UNIVERSITY	62	65	76
MARYLAND, UNIVERSITY OF	175	195	210
MASSACHUSETTS INSTITUTE OF TECHNOLOGY	2125	1713	2382
MASSACHUSETTS, UNIVERSITY OF	85	105	0
MICHIGAN STATE UNIVERSITY	61	61	0
MICHIGAN TECH UNIVERSITY	0	94	105
MICHIGAN, UNIVERSITY OF	129	251	275
MINNESOTA, UNIVERSITY OF	1099	1521	1100
MISSOURI, UNIVERSITY OF	327	180	180

	FY 1983	FY 1984	FY 1985
	(Dollars in Thousands)		
NEVADA, UNIVERSITY OF	78	0	0
NEW MEXICO INST OF MINING TECHNOLOGY	95	0	0
NEW MEXICO, UNIVERSITY OF	95	0	0
NEW YORK CITY U - BROOKLYN COLLEGE	164	90	0
NEW YORK CITY U - CITY COLLEGE	127	91	98
NEW YORK STATE, UNIVERSITY OF ALBANY	5	0	0
NEW YORK STATE, UNIV OF STONY BROOK	850	1081	1480
NORTH CAROLINA A&T STATE UNIVERSITY	50	0	75
NORTH CAROLINA STATE UNIVERSITY	365	240	385
NORTHEASTERN UNIVERSITY	79	100	0
NORTHWESTERN UNIVERSITY	507	210	230
NOTRE DAME, UNIVERSITY OF	90	85	75
OAK RIDGE ASSOCIATED UNIVERSITIES	140	170	200
OHIO STATE UNIVERSITY	244	370	460
OREGON STATE UNIVERSITY	69	85	90
PENNSYLVANIA STATE UNIVERSITY	454	419	696
PENNSYLVANIA, UNIVERSITY OF	372	291	394
PITTSBURGH, UNIVERSITY OF	65	71	75
POLYTECHNIC INSTITUTE, BROOKLYN	75	90	95
PRINCETON UNIVERSITY	73	0	88
PURDUE UNIVERSITY	760	758	903
RENSSELAER POLYTECHNIC	506	593	405
RICE WILLIAM MARSH UNIVERSITY	230	240	285
ROCHESTER, UNIVERSITY OF	187	181	95
RUTGERS UNIVERSITY	189	200	230
SOUTHERN CALIFORNIA, UNIVERSITY OF	251	194	260
SOUTHERN ILLINOIS UNIVERSITY	77	93	100
STANFORD LELAND JR UNIVERSITY	662	589	830
STANFORD UNIVERSITY-SSRL	0	700	1700
STEVENS INSTITUTE OF TECHNOLOGY	84	130	104
SYRACUSE UNIVERSITY	119	0	180
TENNESSEE, UNIVERSITY OF	0	140	0
TEXAS, UNIVERSITY OF	88	115	125
UTAH, UNIVERSITY OF	137	177	289
VIRGINIA POLYTECHNIC INSTITUTE	25	77	87
VIRGINIA, UNIVERSITY OF	237	197	253
WASHINGTON, UNIVERSITY OF	159	180	301
WEST VIRGINIA UNIVERSITY	57	0	65
WISCONSIN, UNIVERSITY OF	313	364	371
OPERATING EXPENSES	21228	20540	25374
CAPITAL EQUIPMENT			
STANFORD UNIVERSITY - SSRL	0	100	300
CAPITAL EQUIPMENT	0	100	300
CONSTRUCTION			
CATHOLIC UNIVERSITY OF AMERICA	0	5000	0
COLUMBIA UNIVERSITY	0	5000	0
NOTRE DAME, UNIVERSITY OF	25	25	0
STANFORD UNIVERSITY-SSRL	0	940	7730
CONSTRUCTION	25	10965	7730
SUBTOTAL	21253	31605	33404

	FY 1983	FY 1984	FY 1985
	(Dollars In Thousands)		
CHEMICAL SCIENCES			
OPERATING EXPENSES			
ALABAMA A&M UNIVERSITY	0	100	0
ALABAMA, UNIVERSITY OF	63	67	71
AMHERST COLLEGE	47	49	50
ARIZONA, UNIVERSITY OF	270	159	254
ARKANSAS, UNIVERSITY OF	0	42	48
BOSTON UNIVERSITY	435	75	272
BRANDEIS UNIVERSITY	90	95	100
BRIGHAM YOUNG UNIVERSITY	251	213	228
BROWN UNIVERSITY	183	209	221
CALIF, UNIVERSITY OF, BERKELEY	0	80	0
CALIF, UNIVERSITY OF, DAVIS	48	82	85
CALIF, UNIVERSITY OF, IRVINE	311	333	350
CALIF, UNIVERSITY OF, LOS ANGELES	287	300	310
CALIF, UNIVERSITY OF, SAN DIEGO	61	64	0
CALIF, UNIVERSITY OF, SANTA BARBARA	265	257	305
CALIFORNIA INSTITUTE OF TECHNOLOGY	268	395	418
CARNEGIE MELLON UNIVERSITY	60	50	0
CHICAGO, UNIVERSITY OF	310	373	309
CLARKSON COLLEGE OF TECHNOLOGY	68	155	0
CLEMSON UNIVERSITY	0	65	0
COLORADO STATE UNIVERSITY	125	138	145
COLORADO, UNIVERSITY OF	264	402	422
COLUMBIA UNIVERSITY	182	410	234
CONNECTICUT, UNIVERSITY OF	51	54	56
CORNELL UNIVERSITY	292	294	295
DARTMOUTH COLLEGE	82	0	41
DREXEL UNIVERSITY	55	60	0
FLORIDA, UNIVERSITY OF	69	71	75
GEORGE WASHINGTON UNIVERSITY	0	58	70
GEORGIA INSTITUTE OF TECHNOLOGY	60	66	70
GEORGIA, UNIVERSITY OF	125	209	208
HARVARD UNIVERSITY	95	100	108
HOUSTON, UNIVERSITY OF	164	258	269
HOWARD UNIVERSITY	45	55	56
ILLINOIS INSTITUTE OF TECHNOLOGY	166	177	190
ILLINOIS, UNIVERSITY OF	165	301	190
INDIANA UNIVERSITY	262	54	209
JACKSON STATE UNIVERSITY	50	55	60
JOHNS HOPKINS UNIVERSITY	146	143	152
KANSAS STATE UNIVERSITY	625	676	734
KANSAS, UNIVERSITY OF	144	154	166
KENT STATE UNIVERSITY	57	66	0
KENTUCKY, UNIVERSITY OF	70	0	0
LEHIGH UNIVERSITY	297	86	115
LOUISIANA STATE UNIVERSITY	70	117	123
MARQUETTE UNIVERSITY	0	60	63
MARYLAND, UNIVERSITY OF	107	0	0
MASSACHUSETTS INSTITUTE OF TECHNOLOGY	724	435	609

	FY 1983	FY 1984	FY 1985
	(Dollars In Thousands)		
MASSACHUSETTS, UNIVERSITY OF	126	0	76
MINNESOTA, UNIVERSITY OF	484	465	389
MISSOURI, UNIVERSITY OF	129	137	149
MOREHOUSE COLLEGE	44	48	0
MOUNT HOLYOKE COLLEGE	0	65	0
NEBRASKA, UNIVERSITY OF	199	283	230
NEW MEXICO, UNIVERSITY OF	90	105	110
NEW ORLEANS, UNIVERSITY OF	55	60	64
NEW YORK CITY U - BROOKLYN COLLEGE	- 5	0	0
NEW YORK CITY U - NEW YORK	80	80	60
NEW YORK STATE, UNIV OF BUFFALO	62	64	68
NEW YORK STATE, UNIV OF STONY BROOK	396	211	330
NEW YORK UNIVERSITY	80	90	90
NORTH CAROLINA, UNIVERSITY OF	305	329	355
NORTHWESTERN UNIVERSITY	155	338	347
NOTRE DAME, UNIVERSITY OF	2663	2835	3005
OHIO STATE UNIVERSITY	140	104	0
OKLAHOMA, UNIVERSITY OF	86	65	63
OREGON GRADUATE CENTER	90	0	70
OREGON, UNIVERSITY OF	29	0	0
PENNSYLVANIA STATE UNIVERSITY	410	486	451
PENNSYLVANIA, UNIVERSITY OF	84	169	179
PITTSBURGH, UNIVERSITY OF	234	221	226
PRINCETON UNIVERSITY	282	309	335
PUERTO RICO, UNIVERSITY OF	125	0	0
PURDUE UNIVERSITY	283	300	331
RENSSELAER POLYTECHNIC	265	85	185
RICE WILLIAM MARSH UNIVERSITY	356	458	275
ROCHESTER, UNIVERSITY OF	185	396	222
RUTGERS UNIVERSITY	5	0	0
SAN DIEGO STATE UNIVERSITY FDT	60	65	68
ST JOHN FISHER COLLEGE	0	60	0
STANFORD LELAND JR UNIVERSITY	402	588	443
SYRACUSE UNIVERSITY	241	324	328
TEMPLE UNIVERSITY	67	80	0
TENNESSEE, UNIVERSITY OF	241	250	256
TEXAS A & M UNIVERSITY	289	226	240
TEXAS TECH UNIVERSITY	112	91	125
TEXAS, UNIVERSITY OF	123	197	137
TOLEDO, UNIVERSITY OF	55	0	32
UTAH, UNIVERSITY OF	379	523	366
VANDERBILT UNIVERSITY	78	82	88
VIRGINIA, UNIVERSITY OF	73	64	67
WASHINGTON STATE UNIVERSITY	0	75	0
WASHINGTON, UNIVERSITY OF	0	70	75
WASHINGTON UNIVERSITY, ST. LOUIS	86	93	90
WAYNE STATE UNIVERSITY	160	160	88
WESLEYAN UNIVERSITY	- 45	0	0
WESTERN MICHIGAN UNIVERSITY	37	55	65
WILLIAM & MARY, COLLEGE OF	75	80	85
WISCONSIN, UNIVERSITY OF	22	191	171

	FY 1983	FY 1984	FY 1985
		(Dollars In Thousands)	
WORCESTER POLYTECH INSTITUTE	43	0	0
WRIGHT STATE UNIVERSITY	55	59	65
WYOMING, UNIVERSITY OF	77	77	81
YALE UNIVERSITY	248	378	408
OPERATING EXPENSES	17824	19153	18569
CAPITAL EQUIPMENT			
NOTRE DAME, UNIVERSITY OF	193	252	359
CAPITAL EQUIPMENT	193	252	359
CONSTRUCTION			
KANSAS STATE UNIVERSITY	0	0	2000
NOTRE DAME, UNIVERSITY OF	25	0	50
CONSTRUCTION	25	0	2050
SUBTOTAL	18042	19405	20978
ENGINEERING, MATHEMATICAL & GEOSCIENCES			
OPERATING EXPENSES			
ALASKA, UNIVERSITY OF	109	120	129
ARIZONA STATE UNIVERSITY	123	0	62
ARIZONA, UNIVERSITY OF	149	110	114
ATLANTA UNIVERSITY	62	67	70
BRIGHAM YOUNG UNIVERSITY	0	20	60
BROWN UNIVERSITY	493	140	281
CALIF, UNIVERSITY OF, BERKELEY	731	293	385
CALIF, UNIVERSITY OF, LOS ANGELES	121	192	72
CALIF, UNIVERSITY OF, SAN DIEGO	0	50	0
CALIF, UNIVERSITY OF, SANTA BARBARA	0	40	0
CALIFORNIA INSTITUTE OF TECHNOLOGY	871	939	1553
CHICAGO, UNIVERSITY OF	203	115	177
CLARKSON COLLEGE OF TECHNOLOGY	88	75	25
COLORADO SCHOOL MINES	80	40	40
COLORADO, UNIVERSITY OF	100	0	100
COLUMBIA UNIVERSITY	626	416	506
CORNELL UNIVERSITY	323	330	270
FLORIDA, UNIVERSITY OF	50	0	0
GEORGE WASHINGTON UNIVERSITY	50	55	60
HARVARD UNIVERSITY	372	0	191
HAWAII, UNIVERSITY OF	96	105	109
ILLINOIS INSTITUTE OF TECHNOLOGY	80	120	100
ILLINOIS, UNIVERSITY OF	414	285	737
INDIANA UNIVERSITY	85	92	90
KENT STATE UNIVERSITY	199	103	108
MARYLAND, UNIVERSITY OF	132	188	196
MASSACHUSETTS INSTITUTE OF TECHNOLOGY	737	926	1500
MASSACHUSETTS, UNIVERSITY OF	0	70	160
MICHIGAN, UNIVERSITY OF	0	60	75
MINNESOTA, UNIVERSITY OF	201	303	332
NEVADA, UNIVERSITY OF	87	95	98

	FY 1983	FY 1984	FY 1985
	(Dollars In Thousands)		
NEW YORK CITY U - CITY COLLEGE	260	150	250
NEW YORK CITY U - QUEENS	49	0	0
NEW YORK STATE, UNIVERSITY OF ALBANY	136	0	62
NEW YORK STATE, UNIV OF STONY BROOK	112	120	124
NEW YORK UNIVERSITY	1800	1930	2250
NORTHWESTERN UNIVERSITY	148	225	59
OREGON, UNIVERSITY OF	103	0	0
PENNSYLVANIA, UNIVERSITY OF	169	142	25
PRINCETON UNIVERSITY	257	0	175
PURDUE UNIVERSITY	60	0	75
RENSSELAER POLYTECHNIC	150	0	98
RICE WILLIAM MARSH UNIVERSITY	249	130	218
ROCKEFELLER UNIVERSITY	53	0	80
SOUTH DAKOTA SCHOOL OF MINES	100	90	93
SOUTHERN CALIFORNIA, UNIVERSITY OF	63	70	0
STANFORD LELAND JR UNIVERSITY	1077	859	1472
STEVENS INSTITUTE OF TECHNOLOGY	0	40	0
TEXAS A & M UNIVERSITY	201	163	155
TEXAS, UNIVERSITY OF	336	98	720
TULSA, UNIVERSITY OF	75	80	82
UTAH, UNIVERSITY OF	120	132	150
VIRGINIA POLYTECHNIC INSTITUTE	142	151	193
WASHINGTON, UNIVERSITY OF	38	40	43
WEST VIRGINIA UNIVERSITY	0	83	0
WISCONSIN, UNIVERSITY OF	177	224	350
WOODS HOLE OCEANOGRAPHY INSTITUTE	190	208	207
YALE UNIVERSITY	88	45	47
OPERATING EXPENSES	12735	10329	14528
CAPITAL EQUIPMENT			
NEW YORK UNIVERSITY	260	200	0
CAPITAL EQUIPMENT	260	200	0
SUBTOTAL	12995	10529	14528
ADVANCED ENERGY PROJECTS			
OPERATING EXPENSES			
CALIFORNIA INSTITUTE OF TECHNOLOGY	238	200	300
CASE WESTERN RESERVE UNIVERSITY	277	300	300
GEORGE WASHINGTON UNIVERSITY	294	300	0
ILLINOIS, UNIVERSITY OF	413	400	200
MASSACHUSETTS INSTITUTE OF TECHNOLOGY	- 14	20	0
NEW MEXICO, UNIVERSITY OF	268	178	400
NORTHEASTERN UNIVERSITY	- 1	0	0
STANFORD LELAND JR UNIVERSITY	- 3	0	0
TUFTS UNIVERSITY	0	154	0
VIRGINIA POLYTECHNIC INSTITUTE	0	48	0
WASHINGTON, UNIVERSITY OF	216	0	300
OPERATING EXPENSES	1688	1600	1500
SUBTOTAL	1688	1600	1500

	FY 1983	FY 1984	FY 1985
	(Dollars in Thousands)		
BIOLOGICAL ENERGY RESEARCH			
OPERATING EXPENSES			
BRANDEIS UNIVERSITY	49	53	57
CALIF, UNIVERSITY OF, BERKELEY	82	85	0
CALIF, UNIVERSITY OF, DAVIS	60	60	0
CALIF, UNIVERSITY OF, IRVINE	134	142	0
CALIF, UNIVERSITY OF, LOS ANGELES	168	87	87
CALIF, UNIVERSITY OF, RIVERSIDE	3	4	0
CALIF, UNIVERSITY OF, SAN DIEGO	50	0	0
COLORADO, UNIVERSITY OF	300	351	0
CORNELL UNIVERSITY	199	163	66
FLORIDA STATE UNIVERSITY	75	0	0
FLORIDA, UNIVERSITY OF	69	0	0
GEORGIA, UNIVERSITY OF	603	571	414
HARVARD UNIVERSITY	120	73	0
IDAHO, UNIVERSITY OF	88	73	75
ILLINOIS, UNIVERSITY OF	450	471	196
INSTITUTE OF PAPER CHEM	31	0	0
IOWA STATE UNIV - AMES	54	0	0
KENTUCKY, UNIVERSITY OF	28	0	71
LEHIGH UNIVERSITY	69	83	0
MARINE BIOLOGICAL LAB	20	0	0
MARYLAND, UNIVERSITY OF	63	64	0
MASSACHUSETTS, UNIVERSITY OF	77	0	0
MICHIGAN STATE UNIVERSITY	1730	1750	1900
MINNESOTA, UNIVERSITY OF	279	178	74
MISSOURI, UNIVERSITY OF	72	67	68
MT SINAI SCHOOL OF MEDICINE	78	73	77
NEBRASKA, UNIVERSITY OF	116	105	0
NEW YORK STATE UNIV OF BINGHAM	90	0	0
NORTH CAROLINA, UNIVERSITY OF	85	87	0
NORTHWESTERN UNIVERSITY	0	60	0
OHIO STATE UNIVERSITY	63	0	0
OKLAHOMA, UNIVERSITY OF	36	47	0
PENNSYLVANIA STATE UNIVERSITY	0	62	0
PENNSYLVANIA, UNIVERSITY OF	80	82	83
PURDUE UNIVERSITY	200	160	80
ROCKEFELLER UNIVERSITY	85	100	0
RUTGERS UNIVERSITY	52	55	0
SOUTHERN ILLINOIS UNIVERSITY	60	62	0
STANFORD LELAND JR UNIVERSITY	143	79	0
UTAH STATE UNIVERSITY	81	70	0
WASHINGTON STATE UNIVERSITY	112	72	0
WASHINGTON, UNIVERSITY OF	205	207	0
WASHINGTON UNIVERSITY, ST LOUIS	133	65	0
WISCONSIN, UNIVERSITY OF	385	320	212
OPERATING EXPENSES	6877	5981	3460
CAPITAL EQUIPMENT			
COLORADO,UNIVBERSITY OF	100	0	0
MICHIGAN STATE UNIVERSITY	150	250	200
CAPITAL EQUIPMENT	250	250	200
SUBTOTAL	7127	6231	3660

5. **For the period FY 1983 - FY 1985, please provide, by BES subprogram and by company, actual and estimated BES funding going to industry.**

Answer: Please see the table for requested information.

BASIC ENERGY SCIENCES

NUCLEAR SCIENCES	FY 1983	FY 1984	FY 1985
	(Dollars in Thousands)		
OPERATING EXPENSES			
ROCKWELL INTERNATIONAL CORP	$ 110	$ 120	$ 120
OPERATING EXPENSES	110	120	120
CAPITAL EQUIPMENT			
ROCKWELL INTERNATIONAL CORP	15	10	0
CAPITAL EQUIPMENT	15	10	0
SUBTOTAL	125	130	120
MATERIALS SCIENCES			
OPERATING EXPENSES			
BATTELLE COLUMBUS LAB	114	160	205
BOEING AEROSPACE CO	75	0	105
HART FRED ASSOC	10	0	0
ROCKWELL INTERNATIONAL CORP	195	140	350
OPERATING EXPENSES	394	300	660
SUBTOTAL	394	300	660
CHEMICAL SCIENCES			
OPERATING EXPENSES			
AEROCHEM RESEARCH LABS, INC.	71	0	0
BEND RESEARCH INC	91	90	93
CALSPAN CORPORATION	49	62	68
OWENS ILLINOIS INC	81	85	90
ROCKWELL INTERNATIONAL CORP	158	0	0
SURFACE ANALYTIC RESEARCH	62	0	0
OPERATING EXPENSES	512	237	251
SUBTOTAL	512	237	251
ENGINEERING, MATHEMATICAL & GEOSCIENCES			
OPERATING EXPENSES			
BATTELLE COLUMBUS LAB	56	56	56
CALSPAN CORPORATION	117	0	0
ELECTROCHEMICAL TECH CORP	69	66	83
FLOW INDUSTRIES INC	0	60	0
GENERAL ATOMIC CO	95	100	25
GEOCHEM RESEARCH	21	109	69
PHYSICAL SCIENCES INC	0	60	0
SCIENCE APPLICATIONS	65	157	75

	FY 1983	FY 1984	FY 1985
	(Dollars in Thousands)		
SCIENTIFIC SYSTEMS	25	0	48
SKF INDUSTRIES	0	100	125
WOODWARD-CLYDE CONSULTANTS	100	110	114
XDATA CORP	65	0	0
OPERATING EXPENSES	613	818	595
SUBTOTAL	613	818	595
ADVANCED ENERGY PROJECTS			
OPERATING EXPENSES			
BEND RESEARCH INC	420	135	600
DYNATECH R/D COMPANY	195	164	200
EIC LABORATORIES	134	142	100
GT DEVICES INC	298	300	0
MATHEMATICAL SCIENCES NW	257	250	150
MEMBRANE TECH & RES INC	84	89	400
NATIONAL TECH SYSTEMS	204	200	300
PHYSICS INTERNATIONAL	494	400	200
RADIATION MONITORING DEVICES	116	120	100
SOLAMAT INC	208	200	200
WESTINGHOUSE R&D CENTER	394	400	100
OPERATING EXPENSES	2804	2400	2350
SUBTOTAL	2804	2400	2350
BIOLOGICAL ENERGY RESEARCH			
OPERATING EXPENSES			
MARTIN MARIETTA CORP	86	95	0
OPERATING EXPENSES	86	95	0
SUBTOTAL	86	95	0

6. **How much of the FY 1985 BES budget request is for support of programs formerly funded by the DOE Nuclear Program and any other DOE Program, such as Magnetic Fusion Energy. Please enumerate these amounts by BES subprogram.**

Answer: Included in the FY 1985 budget request for the Basic Energy Sciences Program is $8.4 million which is associated with program activities formerly funded in the DOE Nuclear Program.

Nuclear Sciences includes $1.4 million associated with nuclear data activities and Chemical Sciences includes $7.0 million which is made up of $2.0 million for GPE responsibility at the Argonne National Laboratory (ANL) and $5.0 million for GPP at ANL.

7. **What level of General Plant Projects (GPP) and General Purpose Equipment (GPE) funding has each of the DOE laboratories received and is expected to receive for the period FY 1983 - FY 1985?**

Answer: The following table identifies the amount of GPP funds provided to the laboratories for the period FY 1983 - FY 1985 and identifies the program providing the funds:

GPP FUNDING BY LABORATORY BY PROGRAM
($ in Thousands)
B/A

	FY 1983	FY 1984	FY 1985
Ames			
Basic Energy Sciences Program.....	$ 275	$ 275	$ 600
Argonne			
Breeder Program..................	500	1,600	0
Basic Energy Sciences Program.....	0[1]	0[1]	5,000
	500	1,600	5,000
Brookhaven			
High Energy Physics Program.......	3,000	3,200	5,700
Idaho National Engineering Laboratory			
Defense Waste Program..............	2,935	4,400	6,455
Lawrence Berkeley Laboratory			
Nuclear Physics Program............	1,500	1,500	2,500
Lawrence Livermore National Laboratory			
Weapons Activities Program.........	4,000	6,000	8,800
Materials Production Program.......	1,100	2,000	0
Biological and Environmental Research Program..................	340	210	250
Magnetic Fusion Program............	1,080	1,000	1,000
Advanced Isotope Separation Program...........................	200	400	500
	6,720	9,610	10,550
Oak Ridge			
Magnetic Fusion Program............	3,500	4,200	7,000
Defense Waste Program..............	2,000	1,870	2,500
	5,500	6,070	9,500
HEDL			
Nuclear Waste Tech Program........	1,000	1,400	1,000
Breeder Program....................	1,500	1,900	4,900
	2,500	3,300	5,900
Pacific Northwest Laboratory			
Biological and Environmental Research..........................	1,100[2]	1,400[2]	2,000
Sandia National Laboratories			
Weapons Activities Program.........	4,000	5,000	7,500
Basic Energy Sciences Program......	-	100	-
	4,000	5,100	7,500

	FY 1983	FY 1984	FY 1985
Savannah River			
Materials Production Program........	2,714	3,133	3,900
Biological and Environmental Research Program..................	50	50	50
Defense Waste Program..............	500	1,740	1,974
	3,264	4,923	5,924
LANL			
Weapons Activities Program..........	4,000	4,350	7,800
Materials Production Program........	0	900	0
Defense Waste Program..............	300	400	300
Nuclear Physics Program............	200	500	950
Biological and Environmental Research Program..................	350	200	250
Magnetic Fusion Program............	420	300	300
-	$5,270	$6,650	$9,600

[1] Prior to FY 1985, the BES program did not have "landlord" responsibility for ANL.

[2] Prior to FY 1985, the BER program did not have "landlord" responsibility for PNL.

The Office of the Controller does not have estimates available of GPE provided to the DOE laboratories so a complete GPE picture is not presented below. However, the following table identifies GPE funds provided to the laboratories by Office of Energy Research Programs only.

GPE FUNDING BY LABORATORY BY PROGRAM
($ in Thousands)
B/A

	FY 1983	FY 1984	FY 1985
Basic Energy Sciences Program			
Ames Laboratory.................	$ 130	$ 140	$ 160
Argonne National Laboratory.....	0[1]	0[1]	2,000
Magnetic Fusion Program			
Oak Ridge National Laboratory...	4,000	4,000	3,600
High Energy Physics Program			
Brookhaven National Laboratory..	3,500	3,500	3,900
Nuclear Physics Program			
Lawrence Berkeley Laboratory....	800	800	800
Biological and Environmental Research Program			
Oak Ridge Associated Universities.	24	30	40
Pacific Northwest Laboratory......	1,200[2]	600[2]	0

[1] Prior to FY 1985, the BES program did not have "landlord" responsibility for ANL.

[2] Prior to FY 1985, the BER program did not have "landlord" responsibility for PNL.

8. **Which DOE programs/subprograms fund GPP and GPE at each of the DOE laboratories?**

Answer: Traditionally GPP funding has been identified in the budget on a total program basis and has not been uniformly separately identified by subprogram. The program amounts by laboratory are reflected in the answer to the question directly preceding this question.

9. **What is the Department doing toward the implementation of recommendations made by (1) the ERAB Multiprogram Laboratory Panel in September 1982, (2) the White House Science Council Laboratory Review Panel (i.e., the Packard Panel) in May 1983, (3) and the President's Private Sector Survey on Cost Control (i.e., the Grace Commission) in December 1983?**

Answer: During the past year the Department has taken several specific actions to improve the overall management of DOE's R&D field operations. These actions are consistent with the recommendations of the Energy Research Advisory Board Laboratory Panel, White House Science Council Laboratory Review Panel and the President's Private Sector Survey on Cost Control. Among the most significant were 1) clarification of the goals of the Department and the missions of its laboratories; 2) development of a comprehensive and uniform annual laboratory appraisal process; 3) establisment of a Department-wide policy on enabling the laboratories to foster innovative exploratory research; and 4) a central Headquarters council to address broad laboratory issues in a timely way.

As recommended in all three reports, the Department's intent is to provide more flexibility, responsibility, and authority to the laboratories and, at the same time, ensure that they are adequately accountable and that their performance is properly evaluated. The Laboratory Management Council, which the Secretary established in September 1983, has already taken several actions aimed at improving the institutional planning process and the general purpose plant needs of the laboratories. In addition, major efforts are also underway to improve the relationship of the laboratories with universities and industry. Finally, the Department also has underway an important management effort aimed at reducing unnecessary and burdensome reporting requirements on the Field to a reasonable level consistent with effective accountability and management.

10. **The January 31, 1984 "Holifield Tables" indicate that the IRB Fiscal Year 1985 budget request for the Basic Energy Sciences (BES) program totalled $418,440,000, including $347,085,000 for operating expenses and $71,355,000 for PACE. According to these tables, the Department's FY 1985 submission to OMB for the program totalled $407,250,000, including $333,410,000 for operating expenses and $73,840,000 for PACE. What are the specific differences between these two budgets?**

Answer: Please see the table below and explanation that follows for the differences between the FY 1985 IRB and the FY 1985 OMB Budget.

(Dollars in thousands)

	FY 1985 IRB Request	FY 1985 OMB Request	Change
Basic Energy Sciences (BES)*			
Materials Sciences			
Operating Expenses..................	$147,210	$140,710	$- 6,500
Capital Equipment..................	15,950	15,450	- 500
Construction.......................	36,000	35,100	- 90
Subtotal..........................	199,160	191,260	- 7,900
Chemical Sciences			
Operating Expenses..................	83,680	85,630	+ 1,950
Capital Equipment..................	7,140	8,840	+ 1,700
Construction.......................	4,900	8,050	+ 3,150
Subtotal..........................	95,720	102,520	+ 6,800
Nuclear Sciences			
Operating Expenses..................	55,155	50,185	- 4,970
Capital Equipment..................	3,620	2,950	- 670
Construction.......................	600	300	- 300
Subtotal..........................	59,375	53,435	- 5,940
Engineering and Geosciences			
Operating Expenses..................	29,000	26,975	- 2,025
Capital Equipment..................	1,825	2,000	+ 175
Subtotal..........................	30,825	28,975	- 1,850
Advanced Energy Projects			
Operating Expenses..................	12,280	10,910	- 1,370
Capital Equipment..................	320	320	0
Subtotal..........................	12,600	11,230	- 1,370
Biological Energy Research			
Operating Expenses..................	14,960	14,800	- 160
Capital Equipment..................	1,000	830	- 170
Subtotal..........................	15,960	15,630	330
Program Direction			
Operating Expenses..................	4,800	4,200	- 600
Subtotal..........................	4,800	4,200	- 600
Total			
Operating Expenses..................	347,085	333,410	-13,675
Capital Equipment..................	29,855	30,390	+ 535
Construction.......................	41,500	43,450	+ 1,950
Basic Energy Sciences................	418,440	407,250	-11,190

*It should be noted that the Applied Mathematical Sciences subprogram was proposed as a separate program, called Energy Science Computational Research (ESCR), with a budget request of $54,145,000, during the OMB budget cycle. It was only after the OMB submission that the decision was made to include this program in Basic Energy Sciences budget. In answer to the next question, the amount included in the BES Congressional Request is reflected.

Explanation of Budget Changes

General

- Budget changes principally the result of meeting OMB target levels. By subprogram the OMB budget reflects the following changes:

Materials Sciences

- A deferral of several new research thrusts
- A general reduction in the Advanced Materials Research Initiative

Chemical Sciences

- The addition of a new initiative in organic chemistry
- The added responsibility for GPE and GPP at Argonne National Laboratory

Nuclear Sciences

- The deferral of the Combustion Research Facility, Phase II
- A general reduction in the activities making up the Nuclear Sciences subprogram, including Nuclear Data, Heavy Ion Fusion, SSRL, Heavy Element Chemistry, and stable and special isotope Production

Engineering and Geosciences

- A deferral of several new research thrusts in Engineering and Geosciences (in computer aided engineering, and Continental Scientific Drilling)

Advanced Energy Projects

- A reduction in the number of projects supported by the subprogram

Biological Energy Research

- A modest share of the general reduction

Program Direction

- A reduction in the staffing level

11. As noted in question 10 above, the Holifield Tables indicated that the OMB FY 1985 budget request for the BES Program totalled $407,250,000, including $333,410,000 for operating expenses and $73,840,000 for PACE. The FY 1985 Congressional request for BES totalled $419,530,000, including $348,340,000 for operating expenses and $71,190,000 for PACE. What are the specific differences between these two budgets?

Answer: Please see the table below and explanation that follows for the differences between the FY 1985 OMB Budget and the FY 1985 Congressional Budget.

(Dollars in thousands)

	FY 1985 OMB Request	FY 1985 Cong. Request	Change
Basic Energy Sciences (BES)			
Materials Sciences			
Operating Expenses.................	$140,710	$141,480	$+ 770
Capital Equipment..................	15,450	15,450	0
Construction.......................	35,100	31,720	-3,380
Subtotal...........................	191,260	188,650	- 2,610
Chemical Sciences			
Operating Expenses.................	85,630	80,930	- 4,700
Capital Equipment..................	8,840	8,840	0
Construction.......................	8,050	8,050	0
Subtotal...........................	102,520	97,820	- 4,700
Nuclear Sciences			
Operating Expenses.................	50,185	49,755	- 430
Capital Equipment..................	2,950	2,950	0
Construction.......................	300	300	0
Subtotal...........................	53,435	53,005	- 430
Applied Mathematical Sciences			
Operating Expenses.................	0	28,250	+28,250
Capital Equipment..................	0	1,500	+ 1,500
Subtotal...........................	0	29,750	+29,750
Engineering and Geosciences			
Operating Expenses.................	26,975	20,795	- 6,180
Capital Equipment..................	2,000	1,500	- 500
Subtotal...........................	28,975	22,295	- 6,680
Advanced Energy Projects			
Operating Expenses.................	10,910	10,810	- 100
Capital Equipment..................	320	320	0
Subtotal...........................	11,230	11,130	- 100
Biological Energy Research			
Operating Expenses.................	14,800	12,490	- 2,310
Capital Equipment..................	830	560	- 270
Subtotal...........................	15,630	13,050	- 2,580
Program Direction			
Operating Expenses.................	4,200	3,830	- 370
Subtotal...........................	4,200	3,830	- 370
Total			
Operating Expenses.................	333,410	348,340	+14,930
Capital Equipment..................	30,390	31,120	+ 730
Construction.......................	43,450	40,070	- 3,380
Basic Energy Sciences..............	407,250	419,530	+12,280

Explanation of Budget Change

General

- Budget changes were principally the result of meeting Administration budget targets. By subprogram the Congressional Budget request reflects the following changes:

Materials Sciences

- Prorata share of the management initiative savings
- The deferral of the Experimental Beam Halls at LANL
- Deferral of funding for the Advanced Light Source with additional funds being made available for research at the SSRL

Chemical Sciences

- The deferral of the new research thrust in catalysis and organic chemistry
- A prorata share of the management initiative savings

Nuclear Sciences

- A prorata share of the management initiative savings

Applied Mathematical Sciences

- The shift of the Energy Science Computational Research program to the BES budget

Engineering and Geosciences

- The deferral of the enhanced research proposed in Continental Scientific Drilling and organic geochemistry
- The deferral of new research thrusts in Mechanical Sciences, Systems Sciences and Engineering Data and Analysis

Advanced Energy Projects

- A minor share of the management initiative savings

Biological Energy Research

- A deferral of the enhanced program proposed in interdisciplinary research

Program Direction

- Management initiative savings and reduction in staffing levels

12. Given the information in questions 10 and 11 above, what are the specific differences between the FY 1985 IRB and Congressional Request budgets for BES?

Answer: Please see table below and explanation that follows for the differences between the FY 1985 IRB and the FY 1985 Congressional Budget.

(Dollars in thousands)

	FY 1985 IRB Request	FY 1985 Cong. Request	Change
Basic Energy Sciences (BES)			
Materials Sciences			
Operating Expenses	$147,210	$141,480	$- 5,730
Capital Equipment	15,950	15,450	- 500
Construction	36,000	31,720	- 4,280
Subtotal	199,160	188,650	-10,510
Chemical Sciences			
Operating Expenses	83,680	80,930	- 2,750
Capital Equipment	7,140	8,840	+ 1,700
Construction	4,900	8,050	+ 3,150
Subtotal	95,720	97,820	+ 2,100
Nuclear Sciences			
Operating Expenses	55,155	49,755	- 5,400
Capital Equipment	3,620	2,950	- 670
Construction	600	300	- 300
Subtotal	59,375	53,005	- 6,370
Applied Mathematical Sciences			
Operating Expenses	0	28,250	+28,250
Capital Equipment	0	1,500	+ 1,500
Subtotal	0	29,750	+29,750
Engineering and Geosciences			
Operating Expenses	29,000	20,795	- 8,205
Capital Equipment	1,825	1,500	- 325
Subtotal	30,825	22,295	- 8,530
Advanced Energy Projects			
Operating Expenses	12,280	10,810	- 1,470
Capital Equipment	320	320	0
Subtotal	12,600	11,130	- 1,470
Biological Energy Research			
Operating Expenses	14,960	12,490	- 2,470
Capital Equipment	1,000	560	- 440
Subtotal	15,960	13,050	- 2,910
Program Direction			
Operating Expenses	4,800	3,830	- 970
Subtotal	4,800	3,830	- 970
Total			
Operating Expenses	347,085	348,340	+ 1,255
Capital Equipment	29,855	31,120	+ 1,265
Construction	41,500	40,070	- 1,430
Basic Energy Sciences	418,440	419,530	+ 1,090

Explanation of Budget Change

General

- The Congressional Budget reflects changes made to reflect Department and OMB priorities and the need to meet overall budget targets. The details by subprogram reflect a combination of the items discussed in detail in the previous Holifield Table answers. As indicated earlier the decision was made after the OMB Budget discussions to include the Energy Science Computational Research program in the BES budget and therefore not have this activity as a separate DOE program.

BES Facilities

13. For the period FY 1983 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, Accelerator and Reactor Improvement and Modification Projects, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to each facility supported totally or partially by the BES program, including the following: (i) Ames Laboratory Materials Preparation Center; (ii) Argonne National Laboratory (ANL) Atomic Spectroscopy Facility; (iii) ANL 4.5-MV Dynamitron Accelerator; (iv) ANL High Voltage Electron Microscope Tandem Facility; (v) ANL Intense Pulsed Neutron Source (IPNS-I); (vi) ANL Premium Coal Sample Program; (vii) ANL Pulse Radiolysis Facility; (viii) Brookhaven National Laboratory (BNL) High Flux Beam Reactor (HFBR); (ix) BNL National Synchrotron Light Source (NSLS); (x) Kansas State University James R. Macdonald Laboratory; (xi) Lawrence Berkeley Laboratory (LBL) National Center for Electron Microscopy; (xii) Los Alamos National Laboratory (LANL) Spallation Neutron Research/Proton Storage Ring (SNR/PSR) Facility; (xiii) Los Alamos Equation of State Library Center; (xiv) Notre Dame Radiation Laboratory (NDRL) Pulse Radiolysis Laboratory; (xv) NDRL Radiolysis-ESR Facility; (xvi) Oak Ridge National Laboratory (ORNL) Electromagnetic Isotope Preparation Facility (Calutrons); (xvii) ORNL EN-Tandem Facility; (xviii) ORNL High Flux Isotope Reactor (HFIR); (xix) ORNL National Center for Small-Angle Scattering Research; (xx) Oak Ridge Electron Linear Accelerator (ORELA); (xxi) ORNL Shared Research Equipment Program (SHaRE); (xxii) ORNL Surface Modification and Characterization Laboratory; (xxiii) ORNL Transuranium Processing Plant (TRU); (xxiv) University Isotope Separator at Oak Ridge (UNISOR); (xxv) Sandia National Laboratories Combustion Research Facility (CRF); (xxvi) Stanford Synchrotron Radiation Laboratory (SSRL); (xxvii) Research Computer Facilities (RCF's); and (xxviii) any additional facilities not identified above. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences. Nuclear Sciences, Advanced Mathematical Sciences, any other BES subprograms, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, Fossil Energy, Conservation, etc.).

Answer: Question 13 concerns 27 centers, facilities or groupings of major equipment that fall into three general categories: 1. User Facilities, 2. Imbedded Facilities -- major equipment or facilities which are part of a research program and are available on limited basis outside the funded project, and 3. centers that are primarily operated to provide a service to the research community.

Thirteen of the facility/centers identified in the question fall into the first category. User facilities are those where facility operating support is provided separately from support for research utilization by the sponsoring DOE subprogram. In most cases, separate Field Task Proposals are submitted by the host laboratory to DOE for facility support. The following facilities fall into this category:

ANL:	High Voltage Electron Microscope Tandem Facility Intense Pulsed Neutron Source

BNL:	High Flux Beam Reactor National Synchrotron Light Source
LBL:	National Center for Electron Microscopy
LANL:	Spallation Neutron Research/Proton Storage Ring
ORNL:	High Flux Isotope Reactor National Center for Small Angle Scattering Research Oak Ridge Electron Linear Accelerator Shared Research Equipment Program Surface Modification and Characterization Laboratory
SNL-L:	Combustion Resarch Facility

Stanford Synchrotron Radiation Laboratory

For each of these, a table has been prepared for insertion into the record providing the detailed information requested. For the purposes of this question, we have used the following definitions:

Operations: This includes costs to operate the facility, providing services to users, whether included under the "in-house" or "out-of-house" definitions below, and other operating expenses identified below.

In-house research: Cost of in-house user research projects, including dedicated equipment. At the IPNS, for example, the support provided by the Materials Sciences subprogram for ANL staff carrying out research using the IPNS meets this definition.

Out-of-house research: Cost to support non-host laboratory researchers using a facility, including dedicated equipment. The source of support may be DOE, other federal agencies, industry, etc. In most cases it can only be estimated although the number of outside users can normally be identified.

Other operating expenses: These include spare parts, "changes in inventory" such as for nuclear reactor fuel elements, and similar items.

Capital equipment: Includes separately budgeted equipment funds provided by BES directly to the facility.

ARIM: Includes BES provided construction funds for accelerator, reactor improvement or modification.

GPP: Funds provided by the responsible program to the host laboratory for general plant projects which are directly related to the facility; BES does not have GPP (or GPE) budget responsibility for any of the laboratories identified in the first category except for ANL beginning in FY 1985.

In-house energy management: BES has no direct involvement in this item; any numbers provided were obtained as information from the laboratories.

I

(iv) Argonne National Laboratory High Voltage Electron Microscope Tandem Facility

	Support Source	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	615	685	750
In-house research	BES/MS	450	500	600
	OTHER	520 E	780 E	860 E
Out-of-house research	BES/MS*	15	20	25
	DOE, OFA INDUSTRY, OTHER	750 E	800 E	1200 E
Capital Equipment	BES/MS	235 E	900 E	925 E
GPP	*	0	200	800

* Numbers provided by Laboratory
E = Laboratory estimate based on number of users and time allotted

II

(v) Argonne National Laboratory Intense Pulsed Neutron Source

	Support Source	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	3895	4712	5066
	INDUSTRY	0	17	30
In-house research	BES/MS	2200	2300	2400
Out-of-house research	BES/MS	400 E	465 E	540 E
	DOE/OTHER	252 E	895 E	982 E
	INDUSTRY	125 E	145 E	170 E
	OFA/NSF	400 E	465 E	540 E
	UNIV.	600 E	700 E	815 E
	FOREIGN	400 E	465 E	540 E
Capital Equipment	BES/MS*	300	275	450
GPP	*	70	25	145

* Numbers provided by Laboratory
E = Laboratory estimate based on number of outside users and time at IPNS

III

(viii) Brookhaven National Laboratory High Flux Beam Reactor

	Support Source	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	6057	6600	7800
In-house research	BES/MS	2698	2900	3200
	BES/CS	410	420	455
	ER/HENP*	1300	826	900
	ER/BER*	624	683	727
Out-of-house research	BES/MS	307 E	330 E	354 E
	OFA	1268 E	1363 E	1464 E
	NON FED	487 E	523 E	563 E
Other operating expenses	BES/MS	200	433	1000
Capital Equipment	BES/MS	200	400	700
	BES/CS	50	60	60
ARIM		0	40	500
GPP	*	66	80	120
In-house energy management	*	285	0	0

* Numbers provided by Laboratory
E = Laboratory estimate based on number of outside users and time at HFBR

IV

(ix) Brookhaven National Laboratory National Synchrotron Light Source

	Support Source	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	5922	7795	8700
	BES/CS	3800	4470	5600
In-house research	BES/MS	1604	1800	2100
	BES/CS	1570	1880	2030
	ER/OTHER	493 E	1303 E	1227 E
Out-of-house research	ER/OTHER	1303 E	2245 E	2690 E
	DOE/OTHER & OFA	1910 E	2160 E	2240 E
	NON-FED	1980 E	3225 E	3960 E
Other operating expenses	BES/MS	250	167	700
Capital Equipment	BES/MS	900	800	800
	BES/CS	770	790	340
ARIM		100 E	600 E	1100 E
GPP		611 E	475 E	700 E
In-house energy management	*	0	0	100 E
Phase II construction	BES/MS	0	2500	10000

* Numbers provided by Laboratory
E = Laboratory estimate based on number of users and time allotted

V

(xi) LBL National Center for Electron Microscopy

	Support Source	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	880	1090	1490
In-house research	BES/MS	500	650	800
Out-of-house research	OTHER	500 E	650 E	800 E
Capital Equipment		300	350	400
Other specific construction projects attributable to this facility		463 E	270 E	100 E

E = Laboratory estimate based on number of outside users and time at NCEM

VI

(xii) Los Alamos National Laboratory Spallation Neutron Research/Proton Storage Ring (SNR/PSR)

	Support Source	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	0	0	500
	DOE/DP*	1450	1600	1700
In-house research	BES/MS	1530	1570	1800
	DOE/DP*	635	800	1165
Capital Equipment	BES/MS	250	300	600
	OTHER*	50	90	100
GPP	*	400	0	0
SNR Improvement project	BES/MS	2700	0	0

* Numbers provided by Laboratory

VII

(xviii) ORNL High Flux Isotope Reactor

	Support Source	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/NS	5590	6150	7820
(Revenue from isotope sales)		644	805	726
(Revenue from other, internal sources for services provided:		383	409	355
In-house research	BES/MS	1868 E	2190 E	2370 E
	ER/OFE	1460 E	1617 E	1545 E
	DOE/NE	583 E	500 E	600 E
Out-of-house research	DOE, OFA, INDUSTRY, OTHER	950 E	720 E	1540 E
	RES EQ*	679 E	720 E	0 E
Other operating expenses	BES/NS	0	0	1450
Capital Equipment	BES/MS	200	400	600
	BES/NS	70	120	80
ARIM		0	0	300 E
GPP		0	0	250 E

* Includes specialized research equipment for use at HFIR and Japanese neutron diffractometer

E = Laboratory estimate based on number of outside users and time at HFIR

VIII

(xix) ORNL National Center for Small-Angle Scattering Research (Center dependent on neutrons produced at HFIR)

	Support Source	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	NSF*	472	466	625
In-house research	NSF*	181	179	241
	BES/MS*	90	90	100
Out-of-house research	DOE, OFA, OTHERS	800 E	800 E	1200 E
Capital Equipment	NSF*	60	100	26

* Estimate by Laboratory of sources of in house support from various projects

E = Laboratory estimate based on number of outside users and time using small angle scattering facility

IX

(xx) Oak Ridge Electron Linear Accelerator (ORELA)

	Support Source	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/NS	1515	1650	1800
In-house research	BES/NS	1422	1510	1700
	INDUSTRY*	200	0	0
	OTHER*	225	0	0
Out-of-house research	BES/NS	90	85	80
Capital Equipment	*	129	240	585
GPP	*	580	0	0

* Numbers provided by Laboratory

X

(xxi) ORNL Shared Research Equipment Program (SHaRE)

	Support Source	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	260	290	320
	BES/OTHER	40 E	45 E	50 E
In-house research*	BES/MS	1292 E	1680 E	1930 E
	ER/MFE	200 E	220 E	250 E
	CONS	75 E	80 E	85 E
	FOSSIL	50 E	60 E	70 E
	NUCLEAR	100 E	50 E	50 E
Out-of-house research	DOE,OFA, INDUSTRY, OTHER	1047 E	1137 E	1195 E
Capital Equipment		57 E	290 E	325 E
ARIM		325 E	0	0

* Estimate by Laboratory of sources of in house support from various projects

E = Laboratory estimate based on number of users and equipment used

XI

(xxii) ORNL Surface Modification and Characterization Laboratory

	Support Source	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	370	500	835
	ER-OTHER	50 E	55 E	60 E
In-house research	BES/MS	865	950	1100
	ER/OFE	125 E	125 E	125 E
	OTHER	305 E	270 E	180 E
Out-of-house research	DOE,OFA, INDUSTRY, OTHER	400 E	400 E	600 E
Capital Equipment		257 E	595 E	825 E
GPP		235 E	650 E	500 E

E = Laboratory estimate based on number of outside users and time at SMCL

XII

(xxv) Sandia National Laboratories Combustion Research Facility

	Support Source	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/CS	2170	2490	2750
In-house research	BES/CS	2160	2290	2500
	BES/OTHER*	1340	1450	1560
	DP*	500	750	1000
	CE*	1450	1650	1900
	OFA/NRC*	330	500	670
	FOSSIL*	1320	1400	1700
Out-of-house research	BES/CS*	680	730	770
	INDUSTRY	40 E	20 E	200 E
Capital Equipment		900	800	700
GPP		0	100	530

* Numbers provided by Laboratory

E = Laboratory estimate based on number of outside users and time at CRF

XIII

(xxvi) Stanford Synchrotron Radiation Laboratory

	Support Source	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations**	BES/NS	5894	6790	7980
Out-of-house research	BES/NS	0	0	0
	BES/MS*	0	800 E	2000 E
	OTHER*	21600 E	33200 E	42900 E
Capital Equipment	BES/NS	456	490	600
GPP		0	0	100
Other specific construction projects attributable to this facility		100 E	2790 E	10130 E

* Numbers provided by Laboratory

** Operated primarily as a user facility

E = Laboratory estimate based on number of outside users, time on SSRL and time at home institutions devoted to preparing experiments, analyzing data

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Eight of the facility/centers fall into the second category of "Imbedded Facilities". They involve specialized pieces of equipment which are central to, and part of, the conduct of a large research project. Their operating costs are usually not separately broken out but are included in the funds provided for the implementation of the research project employing them. The equipment/facility may be made available to qualified users on a case-by-case basis at no cost, when appropriate. The imbedded facility/centers are:

- ANL Atomic Spectroscopy Facility
- ANL 4.5-MV Dynamitron Accelerator
- ANL Pulse Radiolysis Facility
- Kansas State University James R. Macdonald Laboratory
- Notre Dame Radiation Laboratory Pulse Radiolysis Facility
- Notre Dame Radiation Laboratory Radiolysis ESR Facility
- ORNL EN-Tandem Facility
- Research Computer Facilities

The ANL 4.5 MV Dynamitron and the ANL Pulse Radiolysis Facilities are joinly funded by BES and HENP. Accelerator and Reactor Improvement and Modification funds have been provided to these facilities as follows ($K):

	FY 1983	FY 1984	FY 1985
ANL 4.5 MV Dynamitron (Nuc. Physics)	300	100	150
ORNL EN-Tandem Facility	100	100	0

The Kansas State University James R. Macdonald Laboratory is a university-owned atomic physics facility. Research support provided by BES includes funding for operation of an accelerator. Included in the BES FY 1985 request are funds, $2 million, to initiate upgrading of the accelerator at a total estimated cost of $3.4 million to DOE ($1.4 million will be requested to complete the project in FY 1986). Additionally, the State of Kansas will provide $0.6 million to upgrade the housing for the accelerator.

There are 11 Research Computer Facilities, 10 at DOE laboratories and 1 at a university, each consisting of one or more minicomputers dedicated primarily to a specific thrust of the Applied Mathematical Sciences subprogram of BES. Operation of the facilities is supported within the framework of each of the individual projects. Capital equipment funding for these facilities was $800,000 in FY 1983, $970,000 in FY 1984, and the FY 1985 request is for $1.5 million.

Five of the facility/centers fall into the third category. Service facilities generally do not have a research component directly at the facility except to improve the service provided, and operate on a subsidized or cost reimbursable basis. They are listed below and discussed separately.

Ames Laboratory Materials Preparation Center
ANL Premium Coal Sample Bank
LANL Equation of State Library
ORNL Electromagnetic Isotope Preparation Program
ORNL Transuranium Processing Plant

Ames Laboratory Materials Preparation Center
$K

	FY 1983	FY 1984	FY 1985
Operations - Total	892	950	1076
Ames Laboratory Orders	687	740	826
Non Ames Laboratory Orders	205	210	250

The facility operates on a cost reimbursable basis and has no independent facility operating budget. The center consists of special sample preparation apparatus and personnel trained in its use. Samples which are not available from other sources are prepared on order according to specifications on a best effort basis. The center also provides analytical services and acts as a clearing house/referral system for information about the availability of special research samples.

ANL Premium Coal Sample Program
$K

	FY 1983	FY 1984	FY 1985
Operating - Chemical Sciences	454	645	622

The ANL Premium Coal Sample Program collects, prepares and distributes reference grade samples of a small number of representative coals for the use of qualified researchers to establish benchmark experimental measurements in coal science. Exceptionally uniform samples are specially prepared and stored in an inert atmosphere to ensure the chemical stability of the coal over a long period of time.

Los Alamos Equation of State Library
$K

	FY 1983	FY 1984	FY 1985
Operating total	320	350	250
Operating BES - Materials Sciences	120	125	0
Other - Defense Programs	200	225	250

This facility is a computer based Library of Equation of State data and FORTRAN subroutines developed at Los Alamos which are made available without charge to qualified scientists and engineers.

ORNL Electromagnetic Isotope Preparation Facility
$K

	FY 1983	FY 1984	FY 1985
Operating total	3263	3580	5000
Facility	3013	3220	4630
R&D	250	360	370
Operating Source	3263	3580	5000
Isotope Sales	2193	2500	2700
OHER	250	400	600
BES - Nuclear Science	820	680	1700
Capital Equipment			
BES - Nuclear Science	200	500	500
ARIM	0	270	0
GPP	0	100	0

This facility separates stable isotopes for the Research Materials Collection (non consumable).

ORNL Transuranium Processing Plant (TRU)
$K

	FY 1983	FY 1984	FY 1985
Operating total	6182	6378	6749
Separations BES - Nuc. Sciences	4900	5136	5490
Process R&D (NE)	1148	1157	1167
Misc. Reimbursable Services	134	85	92
Capital Equipment BES - Nuc. Sciences	91	95	50

This facility is used to perform two functions. Its principal use is the chemical separation of heavily irradiated target materials for the purpose of preparing research samples of the rare, highly radioactive transuranium elements, none of which occur in nature. A secondary effort is devoted to chemical separations process development funded by the Nuclear Energy program.

14. For the period FY 1983 - FY 1985, by facility and by user, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?

Answer: As noted in the answer to Question 13, several facilities have multiple sources of support which are necessary to meet total operating requirements. Thus, for example, the operation of the Oak Ridge High Flux Isotope Reactor is financed with both programmatic funds and revenues received for service irradiations. Details are shown in the answers in Question 13 for each facility as appropriate.

Materials Sciences Subprogram

15. What is the detailed budget structure of the Materials Sciences subprogram? What types of work are funded by each of these budget categories?

Answer: The Materials Sciences budget is broken down into funds for operating expenses, capital equipment and construction. General plant projects (GPP), Accelerator and Reactor Improvement and Modification projects (ARIM), and prime construction are included under construction. Operating expenses are broken down into three categories which reflect the major disciplines utilized in the program - Metallurgy and Ceramics (01), Solid State Physics (02) and Materials Chemistry (03).

In the (01) metallurgy and ceramics category, research is conducted on the structure of materials, mechanical properties, physical properties, radiation effects and engineering materials by metallurgists and ceramists. The principal aim is to understand the relationship between processing, structure and properties. In this category, researchers study, for example, the microstructure of dual phase steels, fatigue properties of alloys, oxygen diffusion in ceramic oxides, ion irradiation simulation of swelling of stainless steel, and the effect of welding parameters on weld structure and properties.

In the (02) solid state physics category, solid state physicists study the fundamental properties and theory of the condensed state of matter in the areas of neutron scattering, experimental and theoretical solid state physics, particle-solid interactions and engineering physics. Researchers in this category study, for example, the magnetic structure of rare earth compounds using neutron beams, ion implantation and laser annealing, the electronic structure of surface atom layers in elemental catalysts using synchrotron radiation, the theoretical simulation of crystal defects, ion backscattering to understand the fundamental solidification process, and the use of SQUID devices to map magnetic fields.

In the (03) materials chemistry category, chemical structure, high temperature and surface chemistry and engineering chemistry are studied by materials chemists. The objective is to understand the chemical aspects of materials. Researchers in this category study, for example, the chemical structure of one-dimensional organic conductors, the chemical composition of particle surfaces using infra-red spectroscopy, and the use of laser raman scattering to understand surface chemical effects such as corrosion.

Further information on these budget categories and types of research within them is contained in the annual Materials Sciences Programs booklet, the most recent one is for FY 1983, DOE/ER-0143/1. The summary report for this subprogram has been published annually since the early 1960's and has received wide circulation, being announced in technical journals, and is the only complete document of its kind in the Federal government materials research area. This indexed reference document has been of value to both researchers and administrators interested in the content of the Materials Sciences program.

16. For the period FY 1983 - FY 1985, please provide operating expenses, capital equipment, and construction funding for each budget category identified in question 15.

Answer: The funding by year for the Materials Sciences subprogram:

(M$)

Operating	FY 1983	FY 1984	FY 1985
Metallurgy and Ceramics (01)	43.70	48.82	53.27
Solid State Physics (02)	53.40	62.91	73.42
Materials Chemistry (03)	11.06	13.38	14.79
Total Materials Sciences	108.16	125.11	141.48
Equipment*	8.51	12.78	15.45
Construction*	3.00	16.44	31.72

* Equipment and Construction funds are not apportioned by budget category below the subprogram level.

17. For the period FY 1983 - FY 1985. please identify, by budget category and by facility, that portion of Materials Sciences funding going for the support of facilities, such as the National Synchrotron Light Source and other facilities identified in question 13.

Answer: The operating funding for the support of the user facilities identified in question 13:

(K$, Operating)

	Budget Category	FY 1983	FY 1984	FY 1985
LBL				
NCEM	(01)	1380	1750	2200
ANL				
HVEM/TANDEM	(01)	1065	1185	1350
IPNS	(01,02,03)	6095	7012	7466
BNL				
NSLS	(02)	7776	9762	11500
HFBR	(02)	8955	9933	12000
ORNL				
SHaRE	(01)	260	290	320
Neutron Scattering	(02)	1868	2190	2370
Surface Modification	(02)	1235	1450	1935
LANL				
SNR	(02)	1530	1570	2300

Note: When apportioning capital equipment funds to laboratories, the needs of facilities are considered but not specified below the subprogram level.

18. **For the period FY 1983 - FY 1985, please provide, by budget category and by DOE laboratory, the amount of Materials Sciences funding going to DOE laboratories.**

Answer: The funding in Materials Sciences going to DOE Laboratories (in K$):

FY 1983

	Operating Budget Category					
	01	02	03	Total	Equip*	Const*
Ames	2830	2790	1540	7160	760	275
ANL	8020	8090	3830	19940	1670	0
BNL	1850	18880	0	20730	1900	0
INEL	400	0	0	400	40	0
LANL	1180	2300	230	3710	600	2700
LBL	4700	1750	1420	7870	790	0
LLNL	550	730	0	1460	100	0
ORNL	6300	10560	2700	19560	2090	0
PNL	1700	260	0	1960	180	0
SANDIA	2120	1110	0	3230	300	0
SERI	290	60	0	350	30	0

FY 1984

	Operating Budget Category					
	01	02	03	Total	Equip*	Const*
Ames	3000	2910	1610	7520	750	275
ANL	7960	9130	3910	21000	2200	0
BNL	1960	20910	0	22870	1000	640
INEL	500	0	0	500	50	0
LANL	1370	2290	240	3900	650	0
LBL	6120	4410	2770	13300	2550	1760
LLNL	750	770	0	1520	150	0
ORNL	6730	11330	2920	20980	2600	0
PNL	1780	270	0	2050	200	0
SANDIA	2450	1240	410	4100	350	0
SERI	290	130	0	420	100	0
SSRL	0	700	0	700	100	1240

FY 1985

	Operating Budget Category					
	01	02	03	Total	Equip*	Const*
Ames	3120	3080	1700	7900	800	0
ANL	8440	9680	4140	22260	2700	0
BNL	2080	25520	0	27600	1800	11600
INEL	580	0	0	580	60	0
LANL	1460	2780	260	4500	800	0
LBL	7070	5080	3150	15300	2200	10790
LLNL	800	970	0	1770	200	0
ORNL	7150	12950	3100	23200	2900	200
PNL	1790	280	0	2070	250	0
SANDIA	2720	1290	440	4450	490	0
SERI	310	140	0	450	100	0
SSRL	0	1700	0	1700	300	9130

* Capital equipment and construction funds are not apportioned by budget category below the subprogram level.

19. How much of the FY 1985 Materials Sciences budget request is for support of programs formerly funded by the DOE Nuclear Program or by any other DOE program?

Answer: None of the FY 1985 Materials Sciences budget request is for support of programs formerly funded by the DOE Nuclear Program or by any other DOE program.

20. Has the number of materials sciences researchers supported by this subprogram been increasing, stable, or decreasing over the past five years? What change will occur given the FY 1985 budget request?

Answer: The number of materials sciences researchers has decreased about five percent in the period fiscal year 1980-1984. This overall result is the sum of two opposite trends--a significant decrease (in excess of 10 percent) in materials scientists supported at DOE laboratories vs a considerable increase (nearly 10 percent) in university support. Given the fiscal year 1985 budget request coupled with the costs associated with facilities, an additional small (a few percent) reduction in the number of scientists supported will occur, wholly from the DOE laboratories. Overall the number of principal scientists supported in the subprogram has gone from about 900 in FY 1980 to an expected level of slightly over 800 in FY 1985.

21. In the FY 1985 budget request, the Transportation Energy Conservation Program has requested an additional $5.5 million in operating expenses, an increase of 200 percent, for its Advanced Materials Development subprogram; and the Energy Conservation and Utilization Technologies (ECUT) Program has requested an additional $3.7 million, an increase of over 160 percent, for its Materials Sciences Project. How do these activities supplement, complement, or duplicate BES materials research?

Answer: The more technology-focused activities supported by the Advanced Materials Development subprogram of the Transportation Energy Conservation program and by the Materials Project of the Energy Conservation and Utilization Technologies (ECUT) program complement the fundamental research of the BES Division of Materials Sciences. These Energy Conservation programs will help fill a recognized need in the technology programs as pointed out in the ERAB study on materials R&D. The research under the Energy Conservation support will emphasize _processing and processing property measurement_ establishing industrial technology bases needed for advanced energy conversion systems. The research under BES Materials Sciences focuses on _understanding phenomena_ leading to improved properties in materials important to energy technologies. For example, the BES work on the ordered alloy nickel aluminide will investigate fundamental defect structures including grain boundaries as a function of alloy content as well as the role of alloying elements on the resistance of the boundary to deformation and brittle fracture. In contrast, the ECUT work on this compound will gather high temperature stability data of use in design. There is no duplication of efforts in these programs. The programs are coordinated through the DOE Energy Materials Coordinating Committee and the Interagency Group on Ceramic Heat Engines as examples and through contact among the professional staff.

National Research Council Major Materials Facilities Committee

22. What will be the role of the NRC Major Materials Facilities Committee's report in your FY 1986 budget formulation?

Answer: The role of the Committee's recommendations on the DOE budget formulation will be greatly dependent upon the content of the report. BES already provides a wide variety of facilities in the conduct of the DOE research program. These facilities as outlined in question 13 and new national facilities are necessary to maintaining U.S. scientific leadership. The pursuit of the mission of DOE is dependent upon having access to these facilities. The recommendations of the Committee will be reviewed by DOE and discussed with OSTP, NSF, OMB and other agencies, and the DOE mission responsibilities will be examined in light of the recommendations before the FY 86 budget is submitted.

23. Why did OSTP have to go to the National Academy of Sciences for such a study? Isn't this something that DOE should have done?

Answer: DOE is actively participating in the National Academy of Sciences study and, along with NSF, providing financial support. The objective of the study is to examine national facility requirements for all of materials sciences, not just the DOE needs. As an example, the National Bureau of Standards proposal concerned with neutrons is part of the NAS discussion. The National Academy of Sciences provides independent forums for conducting studies of this type. The DOE initially contacted the President of NAS in October 1982 to explore options on the scope and scale of a facilities study. The Seitz Committee is the result.

Advanced Synchroton Radiation Research Planning Study Committee Interim Report

24. In its November 14, 1983 interim report, the Advanced Synchrotron Radiation Research Planning Study Committee recommended as its first priority "expeditious completion of current projects to construct insertion device beamlines at SRC, NSLS and SSRL." What is the Department doing in FY 1984 and expecting to do in FY 1985 to address this recommendation?

Answer: The U.S. Department of Energy is not directly responsible for the development of the facilities at SRC since this is an NSF project and DOE has not received any requests for assistance for such development. The wiggler/undulator technology developed under DOE sponsorship elsewhere will of course be available to SRC. Scientists from LBL have assisted SRC in technical matters with DOE concurrence.

FY 1984 operating funds have been allocated to conduct the necessary research and development for the insertion devices and beamlines associated with the construction of NSLS Phase II. This includes three specific multipole wigglers (a hybrid wiggler for high Q-resolution, a soft x-ray wiggler for x-ray microscopy and holography, and a superconducting wiggler for hard x-ray applications such as medical imaging and invasive chemical techniques) for the x-ray ring and also general consideration of undulators and wigglers for the VUV as well as the x-ray ring. In FY 1985 the Department expects to make available funds to extend this R&D work and to begin construction of these insertion devices at NSLS. These activities and plans are clearly spelled out in the FY 1984 and FY 1985 congressional budget submissions.

The Department's actions in FY 1984 for the expeditious completion of current projects involving insertion devices at SSRL were included in the construction project termed NCAM - which is being reviewed by Congress. FY 1984 operating R&D funds were allocated to support research and development of insertion devices for both SPEAR and the PEP ring - the work is a collaborative effort of SSRL and LBL. FY 1984 construction funds for SSRL when made available will be used for the construction of SPEAR Insertion Device Shielding and the PEP Undulator Beam Line Tunnel and the construction of the associated insertion devices - a 26-period, 2-meter rare-earth cobalt undulator for the PEP ring and a 54-pole rare-earth cobalt wiggler for the SPEAR ring.

For FY 1985 the Department has incorporated a number of the recommendations of the Advanced Synchrotron Radiation Research Planning Study in its request to Congress. For example, the SSRL Enhancement Construction Project has been separated from the LBL CAM project and funding is requested for continuation of this project as well as NSLS-II.

25. **As a second priority, the Committee recommended "the construction of a 6 GeV storage ring beginning in 1987 as a dedicated national facility" with "appropriate R&D funds..allocated in FY85 and FY86." What funding is available in the FY 1985 budget request to support this recommendation?**

Answer: Research and Development operating funds totaling $3.8 M in FY 1985 for research at LBL are requested for generic photon research activities at LBL but none specifically for a 6 GeV storage ring concept. This generic research on undulator/wigglers and beam line optical components, as examples, is important to the improvement of the research capabilities of current synchrotron radiation sources, such as SSRL and NSLS, and as preconstruction R&D for future advanced photon sources. The 6 GeV synchrotron would be such a source.

26. **As its third priority, the Committee recommended "proceeding with the ALS in FY85 as a dedicated national facility." What funding is available in the FY 1985 request to address this recommendation?**

Answer: No construction funds in FY 1985 are requested for this purpose. Decisions on constructing ALS will be made after the report of the NAS Committee on Major Materials Facilities has been completed and reviewed.

27. **The Committee "strongly" recommended "that no action on a lower priority recommendation interfere with the timely pursuit of the higher priority items." Is the Department's FY 1985 request consistent with this recommendation?**

Answer: Our FY 1985 request is completely consistent with this recommendation as reflected in our responses to questions 25 and 26.

28. **Finally, the Committee notes that "rapid developments in synchrotron radiation led the Committee to unanimously recommend that a group such as ours be convened on not less than a yearly basis to review current developments in the entire field and to make recommendations for future actions." Does the Department intend to convene such a group? If so, when, and if not, why not?**

Answer: The Committee report is expected in its final form by the end of March 1984. There are no future plans for this particular committee at this time. The NAS Committee on Major Materials Facilities will complete its report by about June 1984. We will await the conclusions of these two committee reports before making decisions on setting up future external committees. We have set up an interagency coordinating committee on photon sources. We are in sympathy with a continuing committee to coordinate the research and development activities planned by DOE and other agencies but will wait for our review of the conclusions of the above reports.

Advanced Materials Initiative

29. The Department's FY 1984 request for its Advanced Materials Initative totaled $38.0 million, including $28.4 million for construction, $7.7 million for operating expenses, and $1.9 million for capital equipment. Only $3 million was appropriated for construction, but the remainder of the operating and capital equipment funds was appropriated. Please describe in detail the distribution of these funds.

Answer: The following describes the distribution of the FY 1984 appropriations associated with the Advanced Materials Initiative:

(Dollars in Thousands)

	Operating		Equip
SSRL	700	(R&D associated with the SSRL construction project)	100
LBL	2300	(Initiation of research programs in ceramics, electronic materials, catalysis and surface instrumentation, and polymers)	1300
BNL	1000	(R&D associated with construction of and in preparation for NSLS Phase II)	0
LBL	3200	(R&D on generic problems associated with advanced photon systems, vacuum systems, wigglers and undulators, beam line components as part of the newly formed optics center)	500
Contract Research	500	(For new university research associated with advanced photon systems)	0

30. The Department's FY 1985 request for the Advanced Materials Initiative includes $12.55 million for "Programmatic Research and Research and Develoment Associated with Construction." Please describe in detail the plans for the use and distribution of these funds.

Answer: The total for equipment plus operating funds for the Advanced Materials Initiative is only $11.52 million. The plans for the use and distribution of the funds called out for programmatic research and research and development associated with construction are (in K$):

	Operating Funds	Equip. Funds
SSRL	1700 (R&D associated with construction, 700, and materials sciences operations funding at SSRL, 1000)	300
LBL	3800 (Generic R&D on advanced photon systems and beam lines including the optics center research)	700
LBL	2900 (continuation of center for advanced materials research programs on ceramics, catalysis and surface instrumentation, electronic materials, polymers, and an additional effort on alloy deformability)	600
BNL	500 (R&D associated with construction of NSLS Phase II)	0
Contract Research	470 (For university research associated with advanced photon systems)	550
Total	9370	2150

31. **The *ad hoc* Technical Review Panel to Review the Lawrence Berkeley Laboratory Proposal for a National Center for Advanced Materials (NCAM) specifically recommended that final judgement of activities in the areas of Advanced Materials Synthesis and Advanced Device Concepts "be delayed until an acceptable NCAM program plan is available," and that the construction of the Advanced Materials Synthesis Laboratory/Advanced Device Concepts Laboratory (AMSL/ADCL) facility "be deferred until a subsequent review of that plan has been completed." Furthermore, the Panel questioned "whether organizing materials synthesis as a separate, programmatic activity is wise," and suggested "that LBL consider strengthening the materials-synthesis effort in the MMRD, consistent with NCAM's growth." Given the above, why does the FY 1985 budget request include a request for the initiation of funding of the Advanced Materials Laboratory at LBL?**

Answer: The FY 1985 budget construction request includes $1.6 M for the initiation of funding of the Advanced Materials Laboratory (AML). The AML is essential for the success of the Center for Advanced Materials, and would provide needed equipment and space for the focused advanced materials research program, other than surface science and catalysis. The original idea of having a separate synthesis laboratory has been modified taking into account comments and recommendations of the Panel and others during last year's extensive reviews. The timing of this building is consistent with the review panel's recommendation which stated that the building should await an acceptable CAM program plan. A strong effort was undertaken since the Panel report was completed to identify topics, receive industry input and to review the plan and building needs. This has been done by LBL and reviewed and approved by DOE. An Advisory Scientific Policy Board has been established, and an interim Director, Dr. Ken Pitzer, a distinguished scientist has been given responsibility for the evolution of the research program until a permanent Director is named. In view of the progress made to date and the long lead time before the building can be occupied, we believe this request is completely reasonable and essential in order that there be a center for advanced materials research at LBL.

32. **How much funding is provided in each of FY 1983 and FY 1984 for support of the Advanced Light Source (ALS) at LBL? How much support is expected in FY 1985?**

    Answer: The Advanced Light Source (ALS) research was started in FY 1983 with $1.65 million for preconstruction ALS R&D and Source and Optical R&D. It was proposed as a construction project in our FY 1984 budget but no construction funds were appropriated. The program now is being directed in high priority generic R&D problem areas for next generation photon sources and beam line optical components which also will contribute substantially to improving the research capabilities of current facilities such as NSLS and SSRL. Operating funding for this latter activity in FY 1984 is $3.2 million and is planned at a level of $3.8 million in FY 1985. Equipment funding associated with this research program is $0.5 million and $0.7 million in FY 1984 and FY 1985.

Center for Advanced Materials (CAM)

33. **LBL's MMRD trains hundreds of graduate students. What will CAM do to educate and train people in the materials sciences that the MMRD could not do with equivalent resources?**

    Answer: CAM differs substantially in intent from MMRD. Both involve research conducted at the fundamental end of the research and development spectrum of advanced materials technologies. However, each CAM program includes several investigators from different disciplines engaged in a focused activity, whereas MMRD conducts research centered around one faculty investigator and without the explicit industrial interaction required for CAM programs. Also, CAM graduate students will have the opportunity of working with Industrial Fellows on industry related technology.

34. **What is unique about CAM's mission "As an experiment in collaboration between industry and a federal laboratory"? Such collaboration has occurred in other laboratories, such as Oak Ridge, for example.**

    Answer: Uniquely, CAM includes as major participants in its programs visiting scientists from industry and academia along with graduate students, postdoctoral fellows, Berkeley faculty members, and LBL staff scientists.

    At a time when science education is a critical matter for national policy, CAM harnesses one of our nation's strongest centers for scientific education to meet industry's needs for new materials scientists. Hence, the University connection and educational function of CAM yields a different form of collaboration between a Laboratory and Industry.

35. **The MMRD is interdisciplinary. Why can't the MMRD be utilized in much the same way as the National Science Foundation's Materials Research Laboratories to developed focused, interdisciplinary materials research programs?**

    Answer: MMRD is a major national asset, but its personnel and organization are not designed for the mission envisioned for CAM. MMRD has become one of the world's most successful materials and chemical sciences research units by providing stable support for, and encouraging interactions among principal investigators who pursue research topics of their choosing assisted by postdoctoral scientists and graduate students. Some of MMRD's most successful and productive contributors to the advancement of basic science would be unsuited to the more focused, team based basic research carried out in close cooperation with industry. Interactions between MMRD and CAM with their different perspectives and goals, but similar drive for excellence and well-trained, high-caliber scientific staff together should contribute in a significant way to the nation's material science research objectives.

36. **What "novel methods of cooperation and technology transfer between a federal laboratory and industry" is CAM exploring?**

Answer: A major method is the establishment of Industrial Fellowships at CAM. Scientists from industry will work at LBL on CAM projects for a period of 3-12 months. They will bring industrial know-how to the CAM team and will return to their employer with new knowledge of methodology and basic scientific findings in their field. It can be expected that these fellows and their employers will then apply this knowledge to technological applications. In addition, the perspective of these industrial fellows will be a major stimulent to CAM graduate students, who would then be more likely to consider pursuing industrial research careers. Also, the total concept where industrially important topics are selected, workshops held and a Policy Review Board with industrial representatives reporting to the Laboratory Director, is certainly new at Federal Laboratories. This concept can be expected to increase in a significant way technology transfer to the industrial sector of our economy. The most important unique feature of this initiative is the transfer of people - graduate students, industrial fellows and other CAM scientists between the laboratory, industry, and the university.

37. **CAM's stated objectives are "to perform high-quality, industrially responsive materials research, to educate the next generation of scientists and engineers, and to accelerate the translation of basic knowledge into new technology." Couldn't we best accomplish the first and third of these objectives by funding more basic research in which industry is the performer? What is the advantage of having a CAM involved?**

Answer: The Office of Energy Research has responsibility for program guidance as well as substantial programmatic direction for the non-weapons multiprogram laboratories of the Department. There has long been concern that the missions of these laboratories be more responsive to changing requirements, and that their research as well as their facilities become more available and relevant to industrial needs. It is a situation that requires continuing oversight as the requirements of the Department and national needs evolve. The recent reports by the ERAB and the Packard Panel are examples of this oversight.

With this in mind the decision was made to build on the demonstrated research excellence in the basic materials and chemical sciences at LBL. Unique among the national labs was the laboratory's strong connection to and interaction with the faculty and graduate students of the University of California at Berkeley. What CAM adds to this is a programmatic, focussed effort on research established with the advice of industry, and within which industrial collaborators are intended to play a role more intrinsic than being simply users.

CAM's program objectives should not be considered separately from the institutional setting provided by DOE's Lawrence Berkeley Laboratory. By funding the Laboratory, industry in general, rather than one or two corporations, can benefit.

CAM's objectives are also interrelated and should not be considered independently. For example, transferring basic knowledge into new technology happens best by providing industry with minds trained with state-of-the-art equipment on frontier research problems. Traditionally, however, university research is driven by its own internal imperatives. The establishment of CAM at LBL includes the imperatives of industry as well so that the basic research pursued results in skills and knowledge more immediately useful to industry.

In general, industry's basic research efforts are much more targeted than CAM's are intended to be. Industrial research areas are often extremely narrow to correspond with specific market opportunities, and the resource base of manpower and disciplines available in most industrial laboratories is not nearly as broad as that now available at National Laboratories. Building the breadth and depth required for pursuing the activities envisioned for a CAM at a single copany would require an investment of at least the same magnitude as CAM. Even if the investment were spread among several companies, productive use of funds would require that those companies already have a "critical mass" of research and manpower. Indeed, very few companies have that level of investment in research. Thus, federal assistance in the form of this initiative will help small research firms to do adequate research.

38. **In CAM's Electronic Materials Program, the initial thrust is on gallium arsenide. What other gallium arsenide research is being supported by the Materials Sciences subprogram and other DOE programs, such as the Solar Energy program? What gallium arsenide work is being supported by other agencies such as NSF, DARPA, or other parts of DOD, as well as industry?**

Answer: Neither DOE nor NSF presently support any other basic program in the crystal growth and characterization of gallium arsenide, the main initial thrusts of the CAM Electronics Materials Programs.

DARPA and DOD support one experimental crystal growth program at MIT (Professor A. Witt). It focuses on one technique: the Liquid Encapsulated Czochralski (LEC) method. The rest of the GaAs funding goes, primarily to high speed device development, and to industry for some thin-film growth development with standard equipment.

Industry produces GaAs for discrete, standard optoelectronic and switching devices. GaAs crystal growth research and associated development of advanced characterization techniques is vigorously pursued in Japan by Sumitomo and in West Germany by Wacker Chemitronics but not in this country.

39. **How much funding will the Electronics Materials Program receive in each of FY 1984 and FY 1985? Please include operating expenses and capital equiment.**

Answer: Operating expenses are $600,000 for FY 1984 and $740,000 for FY 1985.

The equipment budget is not subdivided by programs since major instruments and equipment are used on more than one program. As indicated earlier in Questions 29 and 30 however, we have separately identified the total equipment funding associated with CAM and the amounts are $1,300,000 for FY 1984 and $600,000 for FY 1985.

40. Please identify specific program milestones for FY 1984, FY 1985, and FY 1986.

Answer: FY 1984:

- An interim crystal growth Laboratory is being installed with the necessary materials handling equipment. Specifically, two Bridgman crystal pullers, 7.5 cm and 12.5 cm diameter, are under procurement and will be operational by August/September 1984.
- A numerical modeling program for heat and mass flow during crystal growth has been fully developed and tested; and it will be adapted to the Bridgman technique to calculate heat flow, temperature distribution, and thermal stresses.
- Conduct GaAs doping experiments specifically aimed at reducing dislocation concentration.
- A research program for the expansion of Lang topography of dislocations in GaAs using synchrotron radiation at SSRL is under development in collaboration with staff at Hewlett-Packard Laboratories.
- A new Electron Paramagnetic Spectrometer is under procurement. This instrument will play a crucial role in the identification and the exploration of the structure of defects in GaAs, specifically the antisite defect.
- A far infrared Fourier transform interferometer shared by many CAM programs will shortly be purchased for the study of shallow and deep level defects in bulk single crystals and thin films of GaAs.
- The Atomic Resolution Microscope (ARM) at LBL's National Center for Electron Microscopy is presently being used to obtain the first atomically resolved pictures of the GaAs lattice.

FY 1985:

- Start-up of routine GaAs crystal growth using Bridgman crystal pullers.
- Characterization methods developed and adapted in FY 1984 will be used for the in-house crystals and will provide direct feedback to improve growth parameters.
- The first results from detailed defect studies can be expected.
- Numerical finite element analysis will be applied to natural convection problems in the melt of the crystal puller.

- Molecular Beam Epitaxy facility at the Department of Electrical Engineering will be expanded to a state-of-the-art, three-chamber system.

FY 1986:

- Crystal purity will be pushed to higher limits. Study of the purity of starting materials, crucibles, and ambient gases together with advanced high-energy SIMS analysis, IR-spectroscopy, EPR and x-ray fluorescence of the GaAs bulk materials will lead to an identification of the major impurity sources.

- The state-of-the-art MBE facility will permit growth of epitaxial films on in-house-grown GaAs substrate. This will permit the study and control of defect and impurity interaction between bulk substrate and epilayer.

- Collaboration with device manufacturers using CAM GaAs will lead to first definitive results on defect-device performance correlations.

41. What unique physical properties of gallium arsenide will CAM explore that other ongoing research is not exploring? What is the uniqueness of the CAM program?

Answer: The uniqueness of the CAM Electronic Materials program lies in the joining of a number of the best scientists and engineers of a National Laboratory, a leading university campus and several companies from throughout the nation to solve the scientific problems which impede the development of advanced high speed, low power consumption devices, electro-optic devices, high speed sensors and digital converters. Initial emphasis is on the growth and characterization of large ($\geq$ 7.5 cm), single-crystals of GaAs, a problem which is not being adequately addressed in this country.

Some physical properties to be studied are:

Critical resolved shear stress at elevated temperatures of single crystals.

Morphology and stability of interfaces between liquid and solid GaAs during crystal growth.

Convection in GaAs melt and in growth ambient.

Real space and electronic structure of the most important shallow and deep level defects.

Defect and impurity interaction between bulk substrate and epitaxial layer.

42. What is the "track record" of the CAM investigators participating in the production, processing, and other aspects of the gallium arsenide research program?

Answer: The initial CAM Electronic Materials Team includes:

W. Hansen (LBL) and E. Haller (LBL and UCB) who have successfully grown the world's purest semiconductors for use in nuclear radiation detector application.

B. Rubinsky (LBL and UCB) who is one of the most successful young theorists in the application of front-tracking finite element analysis.

E. Bourret (LBL) who is a leading expert in the theory and the experiment of compound semiconductor crystal growth. She recently joined CAM, coming from M.I.T.

P. Richards, E. Weber, P. Yu (all LBL and UCB) who are leaders in IR-spectroscopy, deep level studies and pico-second spectroscopy respectively.

R. Gronsky (LBL and UCB) who is one of the world's most outstanding electron microscopists. He is in charge of the atomic resolution microscope at NCEM.

D. Hess and S. Wang (both LBL and UCB) are thin film and epitaxy specialists with experience in industry (Hess) and academic research.

N. Cheung (LBL and UCB), J. Jaklevic (LBL) and N. Amer (LBL) who are leading experts in structural and electronic properties and analysis using Rutherford Backscattering Spectrometry (RBS), x-ray topography and the novel technique of photothermal imaging.

43. What other research in polymer and polymer composites is DOE funding in either the BES Program, Defense Programs, or any other DOE programs, such as the Advanced Gas Centrifuge Program? What polymer and polymer composite research is being supported by other agencies such as the National Science Foundation, and by industry?

Answer: Polymer and polymer composite research is funded by several of the offices of DOE. Except for the fundamental research funded by Basic Energy Sciences, the research is applied, highly specific to certain materials and applications. The CAM research program complements and extends the polymer research funded by Basic Energy Sciences. The topics in CAM were chosen to avoid unnecessary duplication. The National Science Foundation funds research in polymers in the areas of fundamental behavior of synthetic macromolecules; synthesis of new high molecular weight polymers with precisely defined structures; characterization of the chemistry and structure of polymers; molecular arrangements in amorphous and crystalline polymers and mixtures; macromolecular chain dynamics and relaxation, molecular characteristics and their relation to mechanical, optical, transport, surface, and solvent properties; and theoretical treatment of macromolecular behavior. Industrial research in polymers is extensive; however, a large number of industrial consultants were involved in the definition of the CAM program to insure that the research would not duplicate the industrial effort. (See answer to question number 46.)

Examples of Research funded by DOE in polymers and polymer composites are given below by office.

Conservation and Renewable Energy

- Electronic and ionically conducting polymers and battery applications and electrotypic cells.
- Fiber reinforced composites for prototype fly wheels.
- Polymers for energy storage.
- Polymeric solar collectors and cover plates.
- Polymeric seals and gaskets.
- Polymeric membranes for low energy separations.

Military Applications:

- Surface chemistry and bonding of polyaramid fiber reinforced composite.
- Effect of crosslink density on toughness of rubber-modified epoxies.
- Creep-rupture and failure of Kevlar reinforced composites.
- Conducting polymer for electrode materials for high power density batteries and fuel cells.
- Water vapor permeation through elastomer films.
- Super-hard parylene polymer coating development and loading of high-Z metals.
- Low density, microcellular polyolefin foams.
- Evaluation and testing of commercial polymers and adhesives for weapons programs.
- Injection mold process for carbon-fibre reinforced snap-on fittings.
- Composite spring support structures.

Uranium Enrichment and Assessment

- Assessment of commercially available rotor materials for advanced gas centrifuges (test results and materials and classified Restricted Data).

Basic Energy Sciences

- Membrane separations.
- X-ray and neutron scattering to determine polymer structures.
- Degradation and bonding in silver/polymer solar materials.
- Probabilistic models of the stress-rupture of composite materials.

- Analysis of failure modes in short fiber reinforced thermoplastics.
- Structure-property requirements of polymers in mechano-chemical systems.
- Synthesis of water-soluble copolymers and polymers for enhanced oil recovery.
- Corrosion resistant polymer coatings.
- Photophysical studies in pure polymeric films.
- Dynamics of molecular orientation and relaxation in polymers.
- Polymeric ionic and electronic conduction.
- Rubber elasticity.
- Microstructural analysis of ion containing polymers.

44. How much funding will the polymer and polymer composites program receive in each of FY 1984 and FY 1985? Please include operating expenses and capital equipment. What arrangements are being made to take advantage of the unique equipment and facilities at Lawrence Livermore National Laboratory that may be applicable to this program?

Answer: Operating expenses are $360,000 for FY 1984 and $450,000 for FY 1985. Capital equipment is not subdivided by project since major instruments and equipment are used on more than one program. The total equipment funding for CAM is $1,300,000 for FY 1984, $600,000 for FY 1985. A solid state Nuclear Magnetic Resonance unit and a Fourier transform I-R Spectrometer are examples of instruments that will be used on more than one program.

CAM researchers met in December with John Kolb and Richard Christensen from the Composites and Polymers Technology Group at Lawrence Livermore National Laboratory (LLNL) to discuss areas in which the two facilities might interact. LLNL expertise is heavily oriented towards structure/properties work, while CAM research is focused on processing science. The two programs are complementary. LLNL production and development responsibilities are expected to provide the same kinds of stimuli to CAM processing research as the inputs from more traditional industrial laboratories. LLNL synthesis capabilities could be helpful for unusual synthesis needs, otherwise in the future, industrial sources would be more appropriate.

45. Please identify specific program milestones for FY 1984, FY 1985, and FY 1986.

Answer: MILESTONES

FY 1984

- Begin spectral measurements and rheological characterization of polymer liquid crystals.

- Measure flow fields and fiber orientation in fiber filled composites flowing through contractions.
- Begin rheological characterization of block copolymers.
- Elucidate phase compositions of polymer-solvent-nonsolvent systems.
- Initiate theoretical activity and numerical modeling to support all experimental efforts.

FY 1985

- Begin NMR characterization of polymer liquid crystals at various levels of deformation in Mechanical Spectrometer and capillary rheometer.
- Begin measurement of rheology of polyester/glass fiber/small particulate systems.
- Continue rheological characterization of block copolymers.
- Obtain data on velocity field for a single fluid flowing around a sharp corner and two immiscible co-current fluids flowing in a straight channel.
- Complete programming of finite-element computation for co-current flow.
- Prepare membranes under well controlled conditions and examine membrane morphology.
- Complete measurements of fiber orientation and kinematics in contraction and compare with finite-element calculations using continuum theory.
- Develop strategies for molecular weight and composition distribution control in copolymerization.
- Design and construct optical system for rheogoniometer, to detect and measure the characteristics of microstructures found in shear and of those formed at equilibrium but then deformed.
- Incorporation of realistic temperature-dependence in all parameters in final theory of microphase separation, and evaluation of model predictions.
- Begin new theory of block copolymer melt rheology.
- Perform yield-stress measurements with new device, on selected block copolymer melt samples.

FY 1986

- Obtain data on velocity field and interface location for two immiscible fluids in co-current flow around a sharp corner. Examine effect of viscoelasticity, and compare results to finite-element computations.

- Continue NMR characterization of structure development with deformation in liquid crystal polymers.
- Complete rheological characterization of polyester/glass fiber/small particulate systems without crosslinking, and begin study of crosslinking systems.
- Begin theoretical study of spatial development of discontinuities (domains) in Leslie-Ericksen liquid crystal theory.
- Begin theoretical and experimental studies on the influence on solvent-nonsolvent on the morphology evolution in block copolymers and polymer blends.
- Complete the microstructural theory of block copolymer melt rheology.
- Perform rheogoniometer measurement on selected block copolymers to obtain linear and non-linear fluid properties while recording microstructural information with the optical system. Supplement flow data with solid-state characterization of the same samples by electron microscopy and, if available, also by SAXS.

46. How will the CAM polymer and polymer composites program complement, supplement, or duplicate research being conducted at the Polymer Processing Center at the Massachusetts of Technology, the University of Massachusetts-Industry Program on Polymers, and the Center for Applied Polymers at Case Western Reserve University? How many of the industrial sponsors of these centers were consulted in the development of the CAM program in this area?

Answer: The CAM workshop on the program in Polymers and Polymer Composites was attended by representatives of ten major polymer producers and processors, including Dupont, Dow, Celanese, Boeing, Ford, and IBM, as well as representatives of small companies and research laboratories. Most companies represented participated in one or more of the programs at M.I.T., University of Massachusetts, and Case Western Reserve, and in several cases of which we are aware, it was the corporate representatives to these programs who attended the CAM workshop. Numerous other polymer producers and processors were also consulted during the formative period of the program. An advisory group is currently being organized with membership from Dupont, Celenese, IBM and Dow.

The CAM program largely complements the programs at M.I.T., Massachusetts, and Case Western Reserve. As discussed in the response to Question 47, the CAM program focuses on the basic science underlying processing technology in order to develop predictive ability for microstructure distribution. The M.I.T. program focuses on the solution of particular engineering problems related to applications. The University of Massachusetts program emphasizes polymer synthesis and characterization, while the Case Western Reserve program emphasizes structure determination. These are clearly "broad brush stroke" descriptions, and there are elements of all aspects in all programs, but the differences in complementary emphases are real and important.

47. What unique physical properties of polymer and polymer composites are being measured or explored that other ongoing research is not exploring? What is the uniqueness of the CAM program?

Answer: The CAM program focuses on the generic problem of predicting microstructure and microstructure distribution during processing in the fluid state. This is the primary unique emphasis in the CAM program. The general problem requires incorporation of complex fluid rheology, equilibrium thermodynamics, and phase transition kinetics with a description of system geometry, fluid mechanics, heat transfer, mass transfer, and even aerodynamics in the analysis of processing steps such as compression or injection molding and fiber and film extrusion. One example is the prediction of the statistical fiber orientation distribution function and matrix residual stress in the molding of short-fiber polymer composites.

There is general agreement among industrial practitioners, reinforced by the participants at the CAM Polymer and Polymer Composites workshop in October, that there is a pressing need for basic research in the science that underlies advanced polymer and polymer composite processing in order to achieve predictive ability regarding microstructure formation. Such research is not carried out extensively in industry, nor is it a primary focus of the programs mentioned in Question 46.

48. What is the "track record" of the CAM investigators participating in the production, processing, and other aspects of the CAM polymer and polymer composites program?

Answer: Program leader Morton M. Denn has been active in research in polymer processing and rheology for nearly twenty years, during which time he has been an active consultant to major polymer producers and processors. He is the author of four books, numerous book chapters and review papers, and seventy technical papers; more than half of these publications are on subjects relevant to the current CAM program. He is on several major editorial boards. In addition to his industrial consulting, his recognition by industrial practitioners includes the invitation to present the principal lectures at the Third Fiber Producer Conference in 1983. He has been a Guggenheim Fellow (1971-1972) and a Fulbright Lecturer (1979), and presented the William N. Lacey Lectures at Cal Tech in 1979 and the Peter C. Reilly Lectures at Notre Dame in 1980. He was awarded the Professional Progress Award from the American Institute of Chemical Engineers in 1979 "for his incisive investigations into polymer processing and his pioneering studies into process dynamics and control." He has held a Visiting Senior Lecturer position at M.I.T. since 1978, and he was the Visiting Chevron Energy Professor at Cal Tech in 1980.

David S. Soong has been a faculty member at the University of California since 1979, and was promoted to Associate Professor with tenure in 1983. During that time he has published over thirty technical papers on subjects relevent to the CAM program. He is an industrial consultant and a member of the Editorial Advisory Board of the Journal of Polymer Science.

Jeffrey A. Reimer joined the University of California after receiving a Ph.D. in Chemistry at Cal Tech and spending two post-doctoral years at the IBM T.J. Watson Research Center. He is a specialist in Nuclear Magnetic Resonance Spectroscopy, and he was published sixteen technical papers. He was an invited speaker in 1981 at the meeting of the American Physical Society and the 9th International Conference on Liquid and Amorphous Semiconductors.

Michael C. Williams, also on the faculty of the University of California, has been active in research in polymer science and engineering for more than twenty years. He is the author of ninety research papers, approximately two-thirds of which are on subjects relevant to CAM research. He has consulted for industry.

49. Several programs in DOE, including the Materials Sciences subprogram and the Energy Conservation Program, as well as NASA, NSF and other agencies and industry are funding a considerable amount of R&D in ceramics. How does the CAM ceramics program relate to (1) other DOE and other agency ceramics research, and (2) to industrial ceramics research?

Answer: (1) The U.S. research programs in ceramics, funded from all sources, are numerous and varied. Common to all of the programs concerned with ceramic processing and high temperature mechanical properties evaluation is the need to develop a fundamental scientific base. Some large programs, such as those sponsored by NASA and by DOE/Conservation, have mainly ceramics development for ceramic engine demonstration as objectives, and aim to provide a generic technology base. The CAM ceramics program, however, like other science programs of DOE seeks to develop a science data base on which to build the technology. (2) The CAM ceramics program seeks collaborations and interactions with industrial ceramics research efforts, and solicits industrial input to provide assistance on the scope and direction of the CAM-ceramics scientific program through workshops, industrial participation on the Program Advisory Committee, an Industrial Fellows Program, and by exchanging materials and personnel. Similar interactions are offered to the academic community. The industrial programs in this area are mainly funded by the Federal Government and are focused on development of structural ceramics for specific applications.

50. How much funding will the CAM ceramics program receive in each of FY 1984 and FY 1985? Please include operating expenses and capital equipment.

Answer: Operating expenses are $240,000 for FY 1984 and $370,000 for FY 1985. Capital equipment is not subdivided by project since major instruments and equipment are used on more than one program. The total equipment funding for CAM is $1,300,000 for FY 1984, $600,000 for FY 1985.

51. Please identify specific program milestones for FY 1984, FY 1985, and FY 1986.

Answer: MILESTONES

FY 1984

- Hold workshop for program development.
- Initiate organization of fabrication facility.
- Initiate examination of model colloids.
- Initiate powder characterization studies.
- Initiate multiparticle sintering work on 2-dimensional model powders.

- Initiate examination of creep-damage on SiC.

FY 1985

- Scientific equipment for processing of polymeric materials will be installed.
- Examine settling behavior of model colloids by diffraction methods.
- Fabricate silicon nitride powders by gas phase reactions.
- Commence selective baseline study of state-of-the-art silicon nitrides and carbides.
- Examine sintering stresses with loading dilatometer on model powders.
- Initiate development and construction of high temperature-high pressure loading dilatometer.
- Initiate work on high temperature damage model development.
- Initiate work on high temperature erosion and wear experiment.

FY 1986

- Continuation of work in FY 1985 and in addition:
- Initiate fabrication of clean room.
- Complete construction of high temperature-high pressure dilatometer and initiate densification studies on silicon nitride.
- Initiate study of effect of abrasive wear on high temperature mechanical behavior.
- Develop theories on high temperature erosion and wear from observation of damage in elementary erosion and wear events.

52. The CAM Workshop on Advanced Structural Ceramics, originally scheduled for December 1983 was cancelled. What is the basis for the ceramics program being initiated by CAM? How is this program based on specific materials-related "stopper" problems identified by industry?

Answer: The CAM workshop, originally scheduled for December 1983 was postponed since a number of key individuals were unable to attend at that time. The workshop is now scheduled for April 12 and 13, 1984. The CAM ceramics program was deemed suitable, after an LBL and DOE/BES review, to be considered for inclusion in CAM, with a target starting date of February 1, 1984, and with a modest budget permitting further program refinement and development. The scope and approach of the CAM ceramics program has already benefited from extensive discussions with NASA and DOE/Conservation, as well as by various inputs from concerned industries. The incorporation of this input into the program plan is expected to make the April workshop more effective.

The CAM ceramics program is not intended to operate on a task-force basis. As such, it will not directly address industrial "stopper" problems of a short-term nature. Rather, it provides crucial, long term, fundamental research needed to guide development of the next generation of advanced structural ceramics.

53. How does the CAM ceramics program complement, supplement, or duplicate ceramics research being carried out at the Center for Ceramics Research at Rutgers University or at Oak Ridge National Laboratory? How many of the industrial sponsors of the Rutgers' center or researchers at Oak Ridge National Laboratory were consulted as to the content of the CAM program in ceramics?

Answer: Discussions concerning program scope and elimination of overlap were held with J. Wachtman, Director of the Rutgers Center, and with V. Tennery, Ceramic Program Director at the Oak Ridge National Laboratory. As a result of these discussions, every attempt is being made to insure that each of the programs complement one another. Also avenues for collaboration, such as the use of facilities and exchange of materials, have been scoped out.

The workshop document, describing the CAM ceramics program in detail, was distributed to ranking members of 14 companies engaged in fabrication or use of high temperature structural ceramics. A number of these companies are also sponsors of the Rutgers ceramics industrial consortium.

54. What unique physical properties of ceramics are being measured or explored that other ongoing research is not investigating? What is the uniqueness of the CAM ceramics program?

Answer: The CAM ceramics program addresses fundamental scientific questions relating to ceramics fabrication and high temperature properties, such as surface chemistry of ceramic powders, creep-damage accumulation, cyclic loading effects, and erosion and wear in corrosive environments. It explores these properties with a range of unique tools available at LBL, such as atomic resolution electron microscopy, various advanced surface characterization methods, and novel dilatometry techniques.

The CAM ceramics program brings together a group of investigators from different disciplines. It also a very close and productive National Laboratory - University program interaction. A survey of the ongoing research on related subjects in the U.S. has led to an initial program formulation that minimizes overlap with other efforts.

55. What is the "track record" of the CAM investigators participating in the processing, production, and other aspects of the CAM ceramics program?

Answer: At present four senior investigators are involved in the CAM ceramics program. A summary of their vitae is as follows:

Lutgard C. DeJonghe, who is a Staff Senior Scientist at the LBL MMRD, and Associate Professor in Residence, Department of Materials Science and Mineral Engineering, UC Berkeley. Chairman, first Gordon Research Conference on: Science of Ceramic Processing (1981). Editor DOE/BES/Bulletin

"Ceramics: Science of Processing." Editorial subcommittee American Ceramic Society, Electronics Division. Member American Ceramic Society, National Institute of Ceramic Engineers, Ceramic Education Council, Electrochemical Society. 52 refereed journal publications. 2 patents including one patent on a ceramic fabrication technique.

Anthony G. Evans, who is a Faculty Scientist, LBL, MMRD and Professor of Materials Science, Department of Materials Science and Mineral Engineering, UC Berkeley. Chairman Gordon Research Conference on: Mechanical Properties of Ceramics (1978). Editor, Basic Science Division, American Ceramics Society. Associate Editor, Materials Science and Engineering. Member of committees of the National Materials Advisory Board, National Academy of Sciences, National Research Council. Member Materials Research Council Steering Committee. Fellow American Ceramic Society. Member American Institute of Metallurgical Engineers. 110 refereed journal publications.

Ian Finnie, who is Faculty Scientist, LBL, MMRD and Professor and Chairman of Mechnical Engineering Department, UC Berkeley. Member, National Academy of Engineering. Vice President, American Society of Mechanical Engineers. Guggenheim Fellow. Member Institute of Mechanical Engineers (London), American Society for Testing and Materials. 120 refereed journal publications.

Clayton J. Radke, who is Faculty Scientist, LBL and Associate Professor Chemical Engineering, Chemical Engineering Department, UC Berkeley. NSF Senior Fellow. Member American Chemical Society, American Institute of Chemical Engineers, Society of Petroleum Engineers, American Rheological Society. 35 refereed journal publications.

56. A major initial thrust of the advanced surface instrumentation program is to develop a scanning tunneling microscope modeled after a prototype recently developed by IBM in Zurich. What workshops, consultations, etc. were held to choose this program? How is this program based on specific materials-related "stopper" problems identified by industry?

Answer: The program was initiated after detailed, recurring discussions with Binning and Rohrer (IBM Zurich), Wilson (IBM San Jose), Quote (Stanford University), Golovchenko (Bell Labs), and others. Professor Clarke of LBL retains his close relationships with these scientists and will seek to advance the resolution and continuous performances of the device so that it can be utilized in scanning surfaces with a few angstroms resolution. A workshop bringing together these expert workers in this field may be held in the near future when progress warrants.

This surface instrumentation program is for the purpose of enhancing the surface studies and is not an instrumentation development program solely for the sake of instrumentation alone. Two examples of specific problems are: First, an investigation of the surface properties of GaAs, in close collaboration with the GaAs program, in an attempt to shed light on the difficulties of producing a satisfactory oxide layer. Second, a study of the reconstruction of surfaces, in collaboration with the theoretical members of the program, in an attempt to understand the role of this process in the absorption of atomic surface layers and their role in catalysis.

57. Why is it appropriate for DOE to fund CAM for this development? Wouldn't it be more logical to fund IBM directly if DOE wished to have this instrument developed?

Answer: It appears likely that the scanning tunneling microscope (STM) will become a tool of major importance in surface science. As indicated in the answer to Question 56, IBM, Bell Labs, and Stanford University are pursuing the development with their own expertise and do not require DOE assistance. The laboratories are in contact with one another. The device will require many years of investigation, modification, and improvement if its goals are to be achieved. Each of the small groups in the world are employing their own methods, and have their own goals. The goal for CAM is to achieve the ultimate resolution capability using its SQUID expertise in order that this exciting technique can be applied to research problems in the CAM program. With forefront instrumentation such as this, it is not possible to simply buy the instrument or to move the technology to CAM without some ongoing activity.

58. What is the "track record" of the CAM investigators in this program as to the development of advanced surface instrumentation?

Answer: The principal investigator leading the STM project, Prof. J. Clarke, has a 19-year record of very successful development of ultrasensitive instrumentation. He has pioneered the development of the modern SQUID (Superconducting Quantum Interference Device), a device for measuring extremely small magnetic fields, voltages, displacement, etc. This work has lead to the commercial realization of the device by the S.H.E. Corporation. An important energy-related application of SQUIDS, namely remote-reference magnetotellurics (a technique for geophysical surveying) was also pioneered by Clarke. This technology was rapidly transferred to the commercial survey industry and is now almost universally used. This innovation was recognized by the Best Paper Award of the Society of Exploration Geophysicists in 1979, and the "Technology 100" honors list in 1980. Clarke has published about 125 papers on SQUIDS, superconductivity, tunneling, noise and geophysics.

59. What other research in catalysis is DOE funding in either the BES Program, the Fossil Energy Program, or any other program? What catalysis research is being supported by other agencies, such as the NSF, or by industry?

Answer: DOE in BES is funding an appreciable number of catalysis programs. Almost all of the projects are carried out in narrow areas by individual investigators and not by interdisciplinary teams. The CAM Catalysis Program not only contains surface chemists but also synthesis chemists, theoretical physicists and experimental physicists in the fields of superconducting quantum devices and infra-red spectroscopy. This unique combination of scientific disciplines is not found elsewhere. Two of the surface chemists have had a long association with the petroleum industry as either research scientists or consultants. Fossil Energy is primarily funding process development programs, not fundamental long-term research. NSF also supports programs of individual investigations at universities. Petroleum, automotive, and chemical companies have large programs in catalysis. Industrial participation in the workshop on catalysis (see answer to question 62) ensures that the catalysis research at CAM addresses important questions and does not unnecessarily duplicate industrial research.

60. How much funding will the catalysis program receive in each of FY 1984 and FY 1985? Please include operating expenses and capital equipment.

Answer: Operating expenses are $620,000 for FY 1984 and $740,000 for FY 1985. Capital equipment is not subdivided by programs since major instruments and equipment are generally used on more than one program. The total equipment funding for CAM is $1,300,000 for FY 1984, $600,000 for FY 1985.

61. Please identify specific program milestones for FY 1984, FY 1985, and FY 1986.

Answer: MILESTONES:

Zeolites

FY 1984:

- Prepare and characterize two or three zeolites and study variables of synthesis conditions.
- Begin study of nucleation with NMR and Raman Scattering.
- Begin preparation of new zeolites in non-aqueous media.

FY 1985:

- Continue synthesis with major emphasis on nucleation. Use NMR not only for characterization but also to determine effect of templates during synthesis and electron microscopy to study dispersion and location of metals in the zeolite structure.
- Two industrial fellows to join project.

FY 1986

- Explore new routes to zeolite synthesis.
- Investigate the nature of active catalytic sites by model reactions.

Transition Metal Compounds

FY 1984:

- Study preparation of carbides and nitrides of Group IV to VI transition metals and of silicides of Group VIII metals.
- Systematically vary structural chemisorptive and catalytic properties.

FY 1985:

- Begin study of mixed metal compounds or of compounds containing two non-metals, such as carbonitrides and carbosilicides.
- Study low temperature plasma techniques for achieving non-stochiometric compounds with unusual structures.

FY 1986:

- Studies of oxides, sulfides, oxysulfides, and oxycarbides of transition metals are initiated.

Novel Materials and Reaction Conditions in Catalysis

FY 1984:

- Novel organic and metallo-organic monomers will be synthesized with electronic structure tailored to give conducting polymers.
- The immobilization of known polymers capable of binding transition metals on electrodes will be investigated.
- .Catalytic reaction studies of laser and plasma excited molecules will commence.

FY 1985:

- Novel organic and metallo-organic monomers will be subjected to polymerization using initiator chemicals, light or heat.
- The properties of the polymers with respect to solid state and catalytic behavior will be investigated. These systems will affect electron-transfer mediation to and from potential electrocatalysts incorporated in polymer films.
- Model catalytic studies will be initiated.
- The relationship between the excitation energy and excited state distribution of molecules and their reaction selectivity will be explored.

FY 1986:

- Organo-metallic molecules and enzymes will be anchored to polymer surfaces and their catalytic behavior will be investigated.
- The chemical behavior of laser heated and rapidly quenched catalyst surfaces will be explored.

62. How will the CAM catalysis program complement, supplement, or duplicate research being conducted at the MMRD or at other institutions such as the Center for Catalytic Science and Technology at the University of Pittsburgh, the California Institute of Technology, Eastman Kodak Company, UOP, Inc., Mobil Research and Development Company, Exxon Research and Engineering Company, and so on? How many of these performers of catalysis research were consulted in the development of the CAM program in this area?

Answer: The CAM catalysis program concentrates on research in areas other than the programs mentioned in the question. Instrumentation development at CAM would find application in other programs.

Twenty three organizations of the type listed in the question were represented at the workshop for the Catalysis Program, including four of the six explicitly listed. The attendees are listed in the Workshop report. The recommendations of the workshops were incorporated in the proposed research ensuring that the research will complement and extend but not unnecessarily duplicate the research in industries and universities.

63. What unique physical properties of catalysts are being measured or explored that other ongoing research is not investigating? What is the uniqueness of the CAM program?

Answer: The uniqueness of the CAM approach lies in the ability to use many different scientific tools on the same catalyst and catalytic system rather than have various individuals investigate catalysts and systems that differ in composition and operating conditions. The CAM investigations aim to establish the atomic scale properties of catalysts (structure, composition, oxidation states, etc.) and relate them to reaction parameters (rates, selectivities, life-time, methods of synthesis and regeneration). A broad, but focussed program like this requires an interdisciplinary approach that is also unique to CAM. The interdisciplinary approach involves not only surface and catalyst chemists, but also theoretical physicists and experimental physicists who bring new spectroscopies such as scanning tunneling microscopy and high resolution infra-red spectroscopy to bear. The industrial participation in the research is the other important feature.

64. What is the "track record" of the CAM investigators participating in the processing, production, and other aspects of the CAM catalysis program?

Answer: Dr. Gabor Somorjai, who is the leader of the CAM Catalysis Program, Professor of Chemistry of the University of California, Berkeley, is probably the world's most outstanding chemically oriented surface scientist. He is the author of over 300 scientific papers and two textbooks in the fields of Surface Chemistry, Heterogeneous Catalysis and Solid State Chemistry. He is a member of the National Academy of Sciences, a Fellow of the American Physical Society, a Guggenheim Fellow, and has been invited to give numerous distinguished lectureships both in this country and abroad. Dr. Heinz Heinemann who is the deputy leader had a long and distinguished record of catalysis research with Mobil Corporation before coming to LBL.

65. The ad hoc Panel (i.e., the Narath Panel) recommended deferral of the materials synthesis laboratory and instead recommended that LBL consider strengthening the materials synthesis effort in the MMRD "consistent with CAM growth." Given these recommendations, why is CAM requesting funding for an Advanced Materials Laboratory at this early stage?

Answer: The Narath Panel recommended that construction of the AMSL/ADCL building be deferred from FY 1984 until a review of a new program plan has been completed. This has been done and the timing is consistent with the progress made and the long lead time needed for the building completion.

The panel stressed the critical role of new materials in an advanced-materials program and made two important observations that LBL management has seriously considered.

1. The Panel questioned whether organizing materials synthesis in a separate, directed programmatic activity is wise and suggested that "integration of these activities into other CAM programs will be found advantageous."

The Panel's advice to integrate materials synthesis activities into a redefined CAM program was heeded. On November 3, 1983, at the third semiannual review of CAM, DOE was presented a revised CAM program plan consisting of three program areas: Electronic Materials, Structural Materials, and Surface Science and Catalysts. Materials synthesis has been integrated into each new program area. The Surface Science and Catalysis Building will house the Surface Science and Catalysis Program. Together the Electronic Materials and Structural Materials programs constitute a broad Advanced Materials program and would occupy the proposed Advanced Materials Laboratory (AML). The kind and amount of modern laboratory space needed to conduct the Advanced Materials program was presented to DOE at the November review and formed the basis for the FY 1985 request for construction funds.

2. To encourage beneficial interactions between MMRD and CAM and to maintain a balance in materials synthesis research, the Panel suggested that LBL consider strengthening the materials synthesis effort in the MMRD "consistent with CAM growth."

Though it is LBL's intention that the outstanding work in materials synthesis in MMRD will continue, it is of the "basic research push" type described by the Panel, not the "technology-pull" type suitable for CAM. LBL's materials synthesis effort needs to be strengthened in both CAM and MMRD. The additional space and modern facilities of the AML are essential. MMRD research space is fragmented among 13 buildings, none adequate for necessary state-of-the-art synthesis facilities in electronic materials or particle processing.

Chemical Sciences

66. What is the detailed budget structure of the Chemical Sciences subprogram? What types of work are funded by each of these budget categories?

Answer: The Chemical Sciences budget is broken down into funds for operating expenses, capital equipment and construction. General plant projects (GPP) and Accelerator & Reactor Improvement and Modification Projects (ARIM) are included under construction, and general purpose equipment (GPE) under capital equipment. Operating expenses are divided between two budget categories Fundamental Interactions (01) and Processes and Techniques (02).

In the Fundamental Interactions category (01), basic research is supported in photochemical and radiation sciences, chemical physics, and atomic physics. In photochemical and radiation sciences, the photochemical studies are largely devoted to captures of visible light and its conversion to electricity or fuels. Research related to solar photochemical conversion encompasses photoelectrochemistry, homogeneous and heterogeneous redox systems, charge separation in natural photosynthetic systems and in artificial organized assemblies, and photochemistry and photophysics related to solar photoconversion. Radiation chemical studies are conducted on the chemical effects produced by absorption of ionizing radiation and hot atom chemical studies on reactions of highly energetic atoms recoiling from nuclear decay. In chemical physics, the research involves theoretical quantum mechanics, statistical mechanics, chemical dynamics, energy transfer, and molecular structure and spectroscopy. Scientists are investigating the rapid and complex chemical sequences which are fundamental to combustion, using advanced laser diagnostic methods, modeling, and theoretical and kinetic studies of elementary combustion reactions. Research in surface chemistry explores the mechanisms of adsorption, chemisorption and reactions of molcules on catalytic surfaces. The atomic physics program supports expermental and theoretical studies of atom and ion structures, energy levels and lifetimes of quantum states, and of transport and exchange processes involving energy, momentum and matter.

In Processes and Techniques (02), research is supported in chemical energy, separations science, analytical chemistry, and chemical engineering sciences. Chemical energy is rather broadbased, comprising, in the main, research in inorganic, organic and physical chemistry. The emphasis in the chemical energy research is on developing an understanding of the chemical principles underlying technologies related to energy production. These include heterogeneous catalysis, homogeneous catalysis and the chemistry of coal. The separations science and analytical chemistry efforts involve studies of the principles underlying chemical, physical and isotopic separations as well as the development of new analytical techniques. The activities in chemical engineering sciences are the more scientific and energy related aspects of chemical engineering, such as transport phenomna, themodynamics, turbulent flow and rate processes.

A more complete picture of the research supported under these budget categories can be obtained from the annual booklet, Summaries of Research in the Chemical Sciences. The most recent one is for FY 83, DOE/ER-0144/1.

67. For the period FY 1983 - FY 1985, please provide operating expenses, captal equipment, and construction funding for each budget category identified in question 66.

Answer: The funding by year for the Chemical Sciences subprogram is:

	(M$) FY 1983	FY 1984	FY 1985
Operating			
Fundamental Interactions (01)	43.50	46.75	50.66
Processes and Techniques (02)	26.50	28.75	30.27
Total Chemical Sciences	70.00	75.50	80.93
Equipment*	5.51	6.52	8.84[1]
Construction*	0.40	0.45	8.05[2]

[1] Includes $2 M for GPE at ANL.
[2] Includes $5.75 M for GPP, principally at ANL.
* Equipment and Construction funds are not apportioned by budget category below the subprogram level.

68. For the period FY 1983 - FY 1985, please identify, by budget category and by facility, that portion of Chemical Sciences funding going for the support of facilities, such as the National Synchrotron Light Source and other such facilities identified in Question 13.

Answer: Chemical Sciences funds facility operation and research at two major facilities: the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory (in addition to funding of NSLS by Materials Sciences) and the Combustion Research Facility (CRF) at Sandia National Laboratories-Livermore (in addition to funding of research at CRF by other DOE programs). The Chemical Sciences funding at these two facilities is:

	(K$)		
	FY 1983	FY 1984	FY 1985
BNL			
NSLS (01, 02)	5370	6350	7630
SNL-L			
CRF (01, 02)	5010	5510	6020

Note: When apportioning capital equipment funds to laboratories, the needs of facilities are considered but not specified below the subprogram level.

69. For the period FY 1983 - FY 1985, please provide, by budget category and by DOE laboratory, the amount of Chemical Sciences funding going to DOE laboratories.

Answer: The Chemical Sciences funds going to DOE Laboratories are:

FY 1983

	(K$, Operating) Budget Category			(K$)	
	01	02	Total Op.	Equip.*	Const.*
Ames	930	1882	2812	335	0
ANL	7400	3213	10613	885	300
BETC	0	170	170	12	0
BNL	10785	1770	12555	1383	100
INEL	0	165	165	12	0
LANL	0	715	715	52	0
LBL	4296	1740	6036	918	0
LLNL	0	184	184	13	0
MOUND	0	978	978	71	0
NOTRE DAME	2663	0	2663	193	0
ORNL	1640	6085	7725	562	0
PETC	0	80	80	6	0
PNL	0	1300	1300	90	0
SNLA	150	260	410	29	0
SNLL	4790	20	5010	905	0
SERI	450	150	600	44	0

FY 1984

	(K$, Operating) Budget Category			(K$)	
	01	02	Total Op.	Equip.*	Const.*
AMES	910	2036	2946	447	0
ANL	7834	3513	11347	1105	100
BETC	0	177	177	15	0
BNL	11973	1854	13767	1491	0
INEL	0	120	120	11	0
LANL	0	719	719	64	0
LBL	4411	1717	6128	1071	0
LLNL	30	0	30	3	0
MOUND	0	950	950	71	0
NOTRE DAME	2835	0	2835	252	0
ORNL	1658	6058	7716	691	250
PETC	0	93	93	7	0
PNL	0	1310	1310	116	0
SNLA	155	500	655	58	0
SNLL	5280	229	5509	800	100
SERI	575	156	731	65	0

FY 1985

	(K$, Operating) Budget Category			(K$)	
	01	02	Total Op.	Equip.*	Const.*
AMES	925	2205	3130	450	600
ANL	8235	3531	11766	3475	5200
BETC	0	186	186	22	0
BNL	13170	1819	14989	1303	100
INEL	0	126	126	15	0
LANL	0	504	504	60	0
LBL	4455	1670	6125	731	0
LLNL	45	0	45	0	0
MOUND	0	730	730	81	0
NOTRE DAME	3005	0	3005	359	50
ORNL	1725	6206	7931	846	0
PETC	0	87	87	10	0
PNL	0	1419	1419	169	0
SNLA	165	368	533	64	0
SNLL	5750	250	6000	700	0
SERI	675	164	839	100	0
SSRL	0	0	0	0	100

*Capital equipment and construction funds are not apportioned by category below the subprogram level.

70. For the first time in FY 1985, the Chemical Sciences subprogram is funding the General Plant Projects and General Purpose Equipment at Argonne National Laboratory (ANL). What was the rationale for this change?

Answer: It has been the practice of the DOE to assign GPP and GPE funding responsibility for a given laboratory to the program providing the greatest amount of support to that laboratory. In FY 1984 and prior years, the Assistant Secretary for Nuclear Energy's (NE) Breeder Program budgeted these funds for ANL. An analysis of funding trends to ANL prior to the submission of the FY 1983 budget showed declining Breeder Program support to ANL, most of which went to ANL-West, and that the Office of Energy Research's Basic Energy Sciences Program was increasing its support of ANL activities. Thus, the decision was made to transfer funding responsibility to the BES program in 1985 particularly in light of the CRBR cancellation and the general uncertainly regarding breeder funding in the out-years.

71. Please provide a detailed profile of ANL's actual and estimated funding by DOE Program for the period FY 1983 - FY 1985. Please demonstrate conclusively that the Chemical Sciences subprogram provides the majority of ANL's funding.

Answer: The table below identifies funding for ANL for the period FY 1983 - FY 1985 for Nuclear Energy (NE), Office of Energy Research (ER) and other programs. Although the major program at ANL is the Breeder Reactor Systems program (which in the main is carried out at ANL-West) landlord responsibility for ANL resides in the BES program - beginning in FY 1985.

Normally, the predominant program at a particular site, i.e., the single program with the largest amount of funds devoted to that site (breeder in this case), has traditionally been assigned the responsibility to fund GPP and GPE at that site. The predominant program is then referred to as the "landlord" program for that site. An exception to this policy applies to the weapons laboratories where the defense program, although predominant in terms of funding support, only provides for defense program related GPP and GPE. Non-defense related GPP at the weapon laboratories is provided by the appropriate non-defense programs.

It is important to note that predominant program does not mean predominant organization. For example, a particular Assistant Secretary may provide cumulative support, from many programs, to a site which exceeds another Assistant Secretary's cumulative support. However, if the latter provides the greatest funding in a single program, that program becomes the "landlord" for the entire site.

However because of the termination of the CRBR project and the resulting uncertainty in the present, as well as future, budget levels of the breeder program, an exception to the above stated policy was made in assigning ANL "landlord" responsibility. While the breeder program continues to be the single largest program at ANL, a management decision was made by the Laboratory Management Council to assign "landlord" responsibility for ANL to a more stable program, i.e., the BES program, in the interest of reducing GPP/GPE fluctuations and preserving laboratory continuity. However, neither the Chemical Sciences subprogram nor any other BES subprogram provides the majority of funding to ANL.

	FY 1983	FY 1984	FY 1985
NE Total	$ 98.8	$ 98.7	$ 78.9
Operating	88.0	91.2	75.5
Equipment	0.9	3.3	1.8
(GPE Included)	(0.2)	(0.3)	
Construction	9.9	4.2	1.6
(GPP Included)	(0.5)	(1.6)	
ER Total	$ 85.0	$ 83.6	$102.6
Operating	67.1	68.5	73.3
Equipment	6.4	7.1	10.2
(GPE Included)			(2.0)
Construction	11.5	8.0	19.1
(GPE Included)	(7.5)	(7.9)	(13.4)
(GPP Included)			(5.0)
All Other	31.5	26.4	21.5
Total Funding to ANL	$215.3	$208.7	$203.0
Total BES to ANL	($37.9)	($40.0)	($46.1)
Total Chemical Sciences to ANL	($11.8)	($12.6)	($20.4)
(GPE Included)			[($ 2.0)]
(GPP Included)			[($ 5.0)]

Applied Mathematical Sciences

72. We understand that the Department requested over $54 million from OMB for an Energy Science Research Computation Initiative. What is missing in the proposed Applied Mathematical Sciences subprogram that was included in the Energy Science Research Computation Initiative?

Answer: The Energy Science Research Computation (ESRC) initiative to OMB included an increase of $10 million for long range supercomputer research. The Applied Mathematical Sciences subprogram (AMS) request to Congress includes an increase of $6.58 million for long range supercomputer research. The ESRC initiative requested $13.5 million operating funds and $3.35 million capital equipment funds from OMB to support at least three Experimental Computer Facilities, incorporating vendor supplied mainframes with supporting research and development funds for operating systems, languages, etc. These mainframes would include new parallel architectures that show some promise of being the base of supercomputers of the future. The AMS subprogram request to the Congress has no funds for these facilities.

The ESRC initiative requested $4.5 million from OMB to support research on high speed peripherals used with supercomputer systems. The AMS subprogram request to Congress has no funds for this research.

The ESRC initiative included $6 million operating funds and $1.5 million capital equipment funds from OMB for Energy Sciences Advanced Computation. The AMS subprogram request to Congress includes $7 million operating funds and $1.5 million capital equipment funds for this activity. The additional operating funds are included in the request to provide better network access to Energy Research contractors in universities and national laboratories.

73. **The FY 1985 budget justification for this program states that one state-of-the-art supercomputer will be leased to satisfy the computing requirements of the Energy Sciences programs. What type of computer are you planning to lease and where will it be located?**

Answer: Our plan is to lease an enhanced Class VI computer to expand the capacity at the Magnetic Fusion Energy Computer Center (MFECC) at the Lawrence Livermore National Laboratory. Such a machine would satisfy the large scale scientific computing needs of the Energy Sciences programs. Expansion of the MFE Network to accomodate the Energy Sciences represents the lowest cost alternative for providing these programs with high quality supercomputer service in the shortest time.

74. **What cooperative projects among university, DOE laboratory, and industry supercomputer researchers are underway? What such projects are envisioned for the remainder of FY 1984 and in FY 1985?**

Answer: In FY 1984 cooperative projects were underway between Cal Tech and Intel, New York University and IBM, Argonne and Denelcor, Los Alamos and Denelcor, Lawrence Berkeley and Digital Equipment Corporation (DEC), and Lawrence Livermore and DEC.

For the remainder of FY 1984 and in FY 1985, these projects will continue and, in some cases, grow substantially. Potential new projects include participation by the University of Illinois, MIT, Princeton, UC Berkeley, University of Texas, Yale, Purdue, Cornell, Florida State and others, each with industrial partners.

75. **The FY 1985 budget justification says that the long-range research program in large-scale scientific computing will be $21.25 million, an increase of $6.58 million or about 45 percent above FY 1984. How much will be used to fund new proposals?**

Answer: Because most of the existing projects have been funded at a level that provided for theoretical studies of "paper" machines, expansion of these projects to include experimental studies of new architectures will require new proposals for the peer review process. In that sense, almost all of the increase will be used to fund new proposals. The expectation is that more totally new projects can be started in FY 1985, depending upon the quality of the research described in unsolicited proposals that we anticipate will be submitted.

Energy Manpower Assessment

76. What are the reasons for the large increase (+66.7%) in the Energy Manpower Assessment Program for FY 1985 relative to FY 1984?

Answer: The $270K in the FY84 budget for the Manpower Assessment Program (MAP) primarily supports the continued development and updating of a comprehensive energy manpower data base. The purpose of this data base is to provide us with information on current and trend data on the employment and utilization of scientists and engineers in the research, and operation of various energy sources and programs.

The increased budget requested for FY 1985 will enable the MAP to undertake two major activities. First, it will provide the support required to continue the collection and analysis of energy-related scientific and engineering manpower data through NSF-supported surveys (e.g., Ph.D. scientists and engineers in energy R&D and other activities; recent scientists and engineering graduates entering the labor market in energy-related activities). Second, by utilizing the information obtained for the overall energy manpower data base, specific assessments can now be undertaken in various energy areas. For example, because of the shifting trends and activities in the nuclear energy industry, two specific assessments related to nuclear technology developments will be undertaken: an analysis of current occupational employment in nuclear-related activities in private industry and government owned-contractor operated facilities; and, an indepth assessment of manpower supply and demand for selected requirements of the nuclear industry (including the continuing study and analysis of the current and potential supply of new nuclear engineering and health physics/radiation protection graduates required for research, operations, and health and safety activities). Special analyses of the changing patterns of scientific and technical staffing and mobility, and biannual "quick response" surveys of the supply/demand for certain scientific and technical specialists in selected non-nuclear fields would also be carried out as needed.

77. What specific assessments either have been started or are planned to be started in FY 1984 and FY 1985?

Answer: In FY 1984:

- Annual survey of enrollments and degrees in nuclear engineering.
- Annual survey of enrollments and degrees in radiation protection and health physics.
- Follow-up survey of a national sample of experienced scientists and engineers identified in the 1982 Postcensal Survey to determine current involvement in energy work.
- Survey of a national sample of new science and engineering graduates to assess number and characteristics of those in energy work.
- Quick response survey of current labor market conditions for critical specialties in energy industries.

- Annual assessment of employment requirements and manpower supply implications of projected trends in energy R&D and production activities.
- Analysis of employment, education and other characteristics of doctoral scientists and engineers in energy work, 1983.

In FY 1985:

- Survey of occupational employment in nuclear energy activities in private industry and government owned-contractor operated labs and facilities.
- Annual survey of enrollments and degrees in nuclear engineering.
- Annual survey of enrollments and degrees in radiation protection and health physics.
- Indepth assessment of manpower supply and demand for selected segments of the nuclear industry.
- Biennial survey of doctoral scientists and engineers in the workforce involved in energy work.
- Special analysis of the changing patterns of scientific and engineering employment related to shifting energy R&D and production activities.
- Quick response surveys of current labor market conditions for critical scientific and engineering specialties in energy industries.

78. Why does DOE need to support this program, given that similar activities are carried out by the Department of Labor and by the National Science Foundation?

Answer: DOE has a legislative responsibility specifically spelled out in the Energy Reorganization Act of 1974 (and incorporated in the Department of Energy Organization Act of 1977) to help "assure an adequate supply of manpower for the accomplishment of energy research and development programs ... by assuring the collection, analysis and dissemination of necessary manpower supply and demand data."

Although both the Department of Labor and the National Science Foundation carry out activities similar to the manpower assessment programs, neither agency has a mandate or a programmatic interest in supporting studies in specific mission areas (i.e., defense, energy, health, etc.). It is only because DOE has developed a comprehensive energy manpower data base, specifically keyed to a variety of energy technology areas, that the agency has been able to meet various legislated responsibilities in past years (e.g., in areas of nuclear safety research and development, fusion energy, fossil energy). Also, because these assessments are related to specific energy areas, we have been able to provide data to various DOE program areas in developing their long-range program plans and in dealing with manpower training and development.

If DOE were unable to continue conducting these assessments, then both funds and additional personnel slots would have to be alloted to either NSF or Labor to perform the analyses, synthesis and dissemination of energy manpower supply and demand studies required under the referenced legislation. Further, the expertise now extant among DOE staff does not exist elsewhere and would be difficult to replicate by the simple addition of new staff in another agency.

Finally, separation of the manpower assessment function from the energy R&D programs in DOE would lead to duplication of effort, increased costs and increasingly non-useful assessment studies.

General Plants Projects (GPP), General Purpose Equipment (GPE), and Multiprogram General Purpose Facilities (MGPF)

79. Which DOE programs/subprograms fund GPP and GPE at each of the DOE laboratories?

Answer: The following table identifies the programs which provide GPP funds and GPE funds to the laboratories:

PROGRAMS WHICH SUPPORT GPP AT THE LABORATORIES

Ames
- Basic Energy Sciences Program

Argonne
- Breeder Program
- Basic Energy Sciences Program[1]

Brookhaven
- High Energy Physics Program

Idaho National Engineering Laboratory
- Defense Waste Program

Laboratory Berkeley Laboratory
- Nuclear Physics Program

Lawrence Livermore National Laboratory
- Weapons Activities Program
- Materials Production Program
- Biological and Environmental Research Program
- Magnetic Fusion Program
- Advanced Isotope Separation Program

Oak Ridge National Laboratory
- Magnetic Fusion Program
- Defense Waste Program

HEDL
- Nuclear Waste Tech. Program
- Breeder Program

Pacific Northwest Laboratory
- Biological and Environmental Research[2]

Sandia National Laboratories
- Weapons Activities Program
- Basic Energy Sciences Program

Savannah River
- Materials Production Program
- Biological and Environmental Research Program
- Defense Waste Program

LANL
- Weapons Activities Program
- Materials Production Program
- Defense Waste Program
- Nuclear Physics Program
- Biological and Environmental Research Program
- Magnetic Fusion Program

[1] Prior to FY 1985, the BES program did not have "landlord" responsibility for ANL.

[2] Prior to FY 1985, the BER program did not have "landlord" responsibility for PNL.

The Office of the Controller was unable to identify which DOE programs provide GPE support to the laboratories. However, the following table identifies which Office of Energy Research Program provide GPE to the laboratories.

ER PROGRAMS WHICH SUPPORT GPE AT THE LABORATORIES

Basic Energy Sciences Program
- Ames Laboratory
- Argonne National Laborator[3]

Magnetic Fusion Program
- Oak Ridge National Laboratory

High Enegy Physics Program
- Brookhaven National Laboratory

Nuclear Physics Program
- Lawrence Berkeley Laboratory

Biological and Environmental Research Program
- Oak Ridge Associated Universities
- Pacific Northwest Laboratory[4]

[3] Prior to FY 1985, the BES program did not have "landlord" responsibility for ANL.

[4] Prior to FY 1985, the BER program did not have "landlord" responsibility for PNL.

80. How is it decided which DOE program/subprogram funds the GPP and GPE at each DOE laboratory?

Answer: The predominant program at a particular site, i.e., the single program with the largest amount of funds devoted to that site, has traditionally been assigned the responsibility to fund GPP and GPE at that site. The predominant program is then referred to as the "landlord" program for that site. An exception to this policy applies to the weapons laboratories where the defense program, although predominant in terms of funding support, only provides for defense program related GPP and GPE. Non-defense related GPP at the weapon laboratories is provided by the appropriate non-defense programs.

It is important to note that predominant program does not mean predominant organization. For example, a particular Assistant Secretary may provide cumulative support, from many programs, to a site which exceeds another Assistant Secretary's cumulative support. However, if the latter provides the greatest funding in a single program, that program becomes the "landlord" for the entire site.

81. How are the GPP and GPE funding priorities established? What criteria are used?

Answer: While the level of funds budgeted for GPP/GPE is determined by DOE Headquarters, the field offices determine priorities for use of these funds based on general site needs as well as programmatic needs. The GPP data sheets identify samples of projects that will be supported. Generally, GPP and GPE funds are used for the most urgent projects at the time the funds are actually available to the field offices.

GPP projects are intended to be utilized for construction projects totalling less than $1,000,000. During preparation of the FY 1985 budget, the Laboratory Management Council directed that higher funding levels be requested for GPP/GPE in an attempt to maintain the DOE's physical plant assets and to start reversing the current trend of deteriorating facilities. GPE funds are used for equipment of a general site support nature such as fork lifts, lawn mowers, etc.

82. What criteria are used to determine whether or not a given project is to be funded by (a) GPP, (b) the Multiprogram General Purpose Facilities (MGPF) Program, or (c) the In-House Energy Management Program?

Answer: The MGPF program funds only line-item sized projects (i.e. those above $1 million) that benefit two or more programs where no one program uses more than 60% of the facility involved. GPP funds can support any general plant projects with the TEC's less than $1 million. The In-House Energy Management (IHEM) program funds both line-item and GPP sized projects; however, these projects must meet strict payback requirements based on energy cost savings. Payback is only one factor among many considered in the MGPF and GPP programs. Others include safety, health, environment, security, as well as programmatic need and impact.

In general the MGPF program rehabilitates or replaces "multiprogram" facilities when they are deteriorated or constitute a hazard to personnel, operations or other facilities; whereas the IHEM program could replace a given facility if it meets their cost payback criteria (usually 3-5 years). GPP funding levels are established in Headquarters, but, the actual projects undertaken are determined in the field based on a process which determines the highest priority current need each has developed.

83. What centralized management does DOE provide in general, and BES in particular, for the (a) GPP, (b) MPGF Program, and (c) the In-House Energy Management (IHEM) Program?

Answer: All budgets are reviewed in terms of overall levels, issues and interactions at the Assistant Secretary level via the Internal Review Budget and the Institutional Planning processes. The MGPF and IHEM Programs operate agency-wide and their staffs coordinate their budget requests and activities continuously. The IHEM is managed by the Office of Project and Facilities Management, under the Assistant Secretary, Management and Administration. The MGPF Program is managed for the DOE by the Office of Field Operations Management under the Director, Office of Energy Research. The staff a) provides overall program and budget review, b) delegates project execution responsibilities to the Operation's Office and reviews performance periodically, c) does on-site reviews, and d) requests periodic reporting.

The GPP budget is also reviewed on both a Departmental wide basis and also by each of the program offices responsible for managing specific GPP requirements. On a department wide basis GPP levels are reviewed by the Laboratory Management Council. At the program level the individual GPP project requests are reviewed on a more detailed basis both during the formulation and execution phase for each of the projects supported.

84. The January 31, 1984 "Holifield Tables" indicate that the IRB Fiscal Year 1985 budget request for the MGPF Program totalled $60,000,000 for plant and capital equipment (PACE). According to these Tables, the Department's FY 1985 submission to OMB for the program totalled $44,750,000 for PACE. What are the specific differences between these two budgets?

Answer: The following table reflects the projects that were changed from the IRB request to the OMB submission:

($ in Thousands)

Project#	Title	FY 1985 IRB Request	FY 1985 OMB Request	Change
	On-going projects............	$ 21,942	$ 21,942	$ 0
85-R-700	Facility Support, various locations.............	4,991	0	- 4,991
85-R-701	Central Chilled Water Facility, BNL..............	3,500	3,500	0
85-R-702	Replace Laboratory Roofs, ANL........................	4,800	3,300	- 1,500
85-R-703	Primary Electrical Distribution System, ORNL........	2,200	1,100	- 1,100
85-R 704	Rehabilitate Underground Steam System, ANL..........	1,767	3,000	+ 1,233
85-R-705	Electric & Telecommunication System, INEL..........	2,400	708	- 1,692
85-R-706	Medical Facility, LLNL......	2,500	3,400	+ 900
85-R-707	Hanford Site Fire Alarm System Upgrade, HEDL.......	2,800	1,300	- 1,500

($ in Thousands)

Project#	Title	FY 1985 IRB Request	FY 1985 OMB Request	Change
85-R-708	Facility Support, various locations..................	6,400	0	- 6,400
85-R-709	Central Chilled Water Plant, ANL.................	2,500	1,000	- 1,500
85-R-710	Utilities Restoration Piping System, ORNL........	1,500	1,500	0
85-R-711	Upgrade Environmental Monitoring, ORNL...........	1,000	1,000	0
85-R-712	Central Chilled Water System Restoration, ORNL...	1,700	1,000	- 700
85-R-713	Replace Transportation Complex, INEL..............	0	2,000	+2,000
	Total MGPF...............	$ 60,000	$ 44,750	$-15,250

85. As noted in question 84 above, the Holifield Tables indicated that the OMB FY 1985 budget request for the MGPF totalled $44,750,000 for PACE. The FY 1985 Congressional request for MGPF totalled $38,950,000 for PACE. What are the specific differences between these two budgets?

Answer: The following table reflects the projects that were changed from the OMB Request to the Congressional submission:

($ in Thousands)

Project#	Title	FY 1985 OMB Request	FY 1985 Cong Request	Change
	On-going projects............	$ 21,942	$ 21,942	$ 0
85-R-701	Central Chilled Water Facility, BNL...............	3,500	3,500	0
85-R-702	Replace Laboratory Roofs, ANL.........................	3,300	3,508	+ 208
85-R-703	Primary Electrical Distribution System, ORNL.........	1,100	1,100	0
85-R 704	Rehabilitate Underground Steam System, ANL...........	3,000	3,000	0
85-R-705	Electric & Telecommunication System, INEL...........	708	0	- 708
85-R-706	Medical Facility, LLNL.......	3,400	1,600	- 1,800
85-R-707	Hanford Site Fire Alarm System Upgrade, HEDL........	1,300	1,300	0
85-R-709	Central Chilled Water Plant, ANL..................	1,000	1,000	0
85-R-710	Utilities Restoration Piping System, ORNL.........	1,500	0	- 1,500
85-R-711	Upgrade Environmental Monitoring, ORNL............	1,000	1,000	0
85-R-712	Central Chilled Water System Restoration, ORNL ...	1,000	1,000	0
85-R-713	Replace Transportation Complex, INEL...............	2,000	0	- 2,000
	Total MGPF..................	$ 44,750	$ 38,950	$- 5,800

86. Given the information in questions 84 and 85 above, what are the specific differences between the FY 1985 IRB and Congressional Request budgets for MGPF?

Answer: The following table reflects the projects that were changed from the IRB Request to the Congressional submission:

($ in Thousands)

Project#	Title	FY 1985 IRB Request	FY 1985 Cong Request	Change
	On-going projects............	$ 21,942	$ 21,942	$ 0
85-R-700	Facility Support, various locations....................	4,991	0	- 4,991
85-R-701	Central Chilled Water Facility, BNL...............	3,500	3,500	0
85-R-702	Replace Laboratory Roofs, ANL...........................	4,800	3,508	- 1,292
85-R-703	Primary Electrical Distribution System, ORNL.........	2,200	1,100	- 1,100
85-R 704	Rehabilitate Underground Steam System, ANL...........	1,767	3,000	+ 1,233
85-R-705	Electric & Telecommunication System, INEL...........	2,400	0	- 2,400
85-R-706	Medical Facility, LLNL.......	2,500	1,600	- 900
85-R-707	Hanford Site Fire Alarm System Upgrade, HEDL........	2,800	1,300	- 1,500
85-R-708	Facility Support, various locations....................	6,400	0	- 6,400
85-R-709	Central Chilled Water Plant, ANL..................	2,500	1,000	- 1,500
85-R-710	Utilities Restoration Piping System, ORNL.........	1,500	0	- 1,500
85-R-711	Upgrade Environmental Monitoring, ORNL............	1,000	1,000	0
85-R-712	Central Chilled Water System Restoration, ORNL....	1,700	1,000	- 700
	Total MGPF..................	$ 60,000	$ 38,950	$-21,050

Small Business Innovative Research (SBIR) Program

87. How much has the BES Program contributed to the support of DOE's Small Business Innovative Research (SBIR) Program for FY 1983? How much is estimated for FY 1984 and FY 1985? How was this assessment determined?

Answer: The BES Program contributed $537,000 to the SBIR program in FY 1983 and we estimate that $1,740,000 and $3,445,000 will be contributed in FY 1984 and FY 1985, respectively. The assessment was based on the amount of extramural research conducted by the BES Program and was applied by year according to the percentages specified in the legislation (0.2%, 0.6%, 1.0% and 1.25%, respectively).

88. What level of funding will be available for the SBIR program in FY 1984 and in FY 1985? How many awards do your expect to award in each of FY 1984 and FY 1985?

Answer: Based on the Congressional budget, we project that $15,800,000 and $26,000,000 will be made available to the SBIR Program in FY 1984 and FY 1985. With this level of support we project the number of awards at around 100 Phase I awards and around 50 first year Phase II awards in FY 1984. In FY 1985 we project the number of awards at around 100 Phase I and around 50 new Phase II awards. In FY 1985 we will also be providing the second year funding for the Phase II awards made in FY 1984 as specified in the legislation.

Management Initiatives

89. According to the BES budget justification (Congressional Budget Request, FY 1985, Volume 3, p. 145), the FY 1985 budget request of $419,530,000 reflects $3,000,000 for savings resulting from management initiatives in the area of administrative processes/field structure. What specific initiatives will result in these savings?

Answer: This management initiative is one of several initiatives which reflect the first implementation efforts of the DOE with regard to recommendations contained in various studies of departmental operations, including the President's Private Sector Survey on Cost Control (The Grace Commission) and the Federal Laboratory Panel of the White House Science Council (The Packard Report), as well as the Administration's program for improved management systems known as Reform 88.

The $3,000,000 in the BES program represents savings in FY 1985 resulting from improved management of government owned, contractor operated (GOCO) facilities. This initiative involves improved utilization of private sector business practices by GOCO contractors through reduced procedural controls and heightened reliance on policy issuances and performance evaluation by the DOE Operations Offices. Cost initiatives for improved GOCO performance and reduction in reporting detail will lead to DOE management oversight at a higher level and to improved opportunities for innovation and implementation of new management processes by GOCO contractors. These savings will occur at all eight DOE operations offices and major contractors.

90. Who will determine how these specific initiatives result in these savings?

Answer: These initiatives will involve a wide variety of activities including a thorough examination of reporting requirements and reductions in those requirements and a thorough examination of procedural requirements levied on our contractors in such areas of achievements of socioeconomic procurement goals, management of subcontractor activities, program and management planning activities and others. In each case the principal staff or program office responsible for the activity being examined will be required to identify savings opportunities and initiate the actions to implement those activities. For example: reduction in procurement reporting requirements would be directed by the Procurement Office, reduction in ADP reporting by the Office of ADP Management and so forth. The overall effort will be coordinated and results will be assessed by the Assistant Secretary for Management and Administration.

91. How will these savings be apportioned among the DOE Operations Offices, laboratories, and other contractors?

Answer: All field offices and GOCO contractors will be expected to contribute efforts to achieve these savings. The impact on any individual organization will depend upon DOE assessment of the collective affect of eliminating or consolidating reporting requirements or simplifying procedures. For example: If a particular organization has estimated that meeting a particular reporting requirement requires four staff years of effort and that requirement is eliminated, DOE would expect the organization in question could reduce their overhead staffing by four staff years. While the data for making these estimates are not precise we believe it is sufficient to arrive at a reasonable basis to allocate the resultant savings without adverse impact on programmatic activities.

Minority Questions for Dr. Trivelpiece

Supporting Research and Technical Analysis

February 23, 1984

1. **In the Applied Mathematical Sciences program the request is made for $21.25 million to expand scientific computing research.**

   What amount will be used to acquire hardware and software for data processing? for computing research?

   To what extent will industry be involved in computing research as consultant? participant? supplier?

   Answer: The $21.25 million for operating funds for supercomputer research in the Applied Mathematical Sciences subprogram is intended to support basic research in three categories: (1) Analytical and Numerical Methods - includes physical and computational mathematics focused on numerical methods for solving systems of partial differential equations used in modeling complex energy systems; (2) Information Analysis Techniques - includes computational statistics and data management techniques for analyzing very large scientific data sets common to many DOE programs; and (3) Advanced Computing Techniques - includes software engineering techniques and algorithmic studies focused on novel parallel computer architectures. The only hardware acquired from this budget will be equipment requested in unsolicited research proposals from universities and private research firms. Hardware for DOE laboratories is budgeted under capital equipment and is described in that section of the budget.

   Because the program is administered on the basis of acceptance of peer reviewed unsolicited research proposals, no definitive dollar allocations can be stated until the program is underway, in mid FY 1985. However, there are several examples of university/industry/laboratory collaborations already being supported in FY 1984. One example is the NYU/IBM collaboration in which IBM is participating with NYU in designing the NYU Ultracomputer. So far, IBM has supplied a small amount of funds to NYU to complement the research support from DOE. Another example is the Cal Tech project in which Intel agreed to supply the processor chips and DEC has donated some minicomputers. DOE is funding a major portion of the work in algorithm design and problem decomposition in areas such as high energy physics, geophysics, chemistry, as examples. Other examples are the cooperative agreements between Denelcor and LANL and between Denelcor and ANL, in which discounts and maintenance support for the Denelcor HEP-1 machine were negotiated. These machines are used for research in parallel algorithms for DOE problems that must be completely restructured for the new architecture. It is anticipated that many good research proposals involving university/laboratory/industry collaboration will be received in the next few years. The traditional roles will be maintained: universities provide many innovative ideas and train graduate students in the design and use of large scale scientific computers; DOE laboratories have superior expertise in solving real-world problems in supercomputing and provide positions for postdoctoral students; and industry excels in implementing hardware designs as well as benefitting directly from the transfer of technology from the research environment.

2. **You appear to be embarked on a continuing scientific computing research program. What has motivated this action? How long will it take? How much will it cost? Who will be involved?**

Answer: The Applied Mathematical Sciences research subprogram evolved from a program started in approximately 1952. At the suggestion of AEC Commissioner John von Neumann, Dr. John Pasta was asked to start a program in computational research because of the obvious requirements of the Manhattan project and its follow on activities at Los Alamos. One of the first actions of the program was the installation of the Univac computer at NYU to provide unclassified access to AEC researchers. Since 1970 the program has been supported at a relatively constant level of effort. The expanded program for FY 1985 is the outgrowth of a series of studies done over the last few years on new advanced computational approaches that culminated in the Lax Report and the Federal Coordinating Council for Science, Engineering and Technology (FCCSET) studies. DOE has traditionally invested a major effort in scientific computation in weapons design, magnetic fusion, and, more recently, in fundamental physics and chemistry studies.

The program can be viewed as having an intermediate term goal and a long term goal. Work supported by the program over the last three decades has been focused on designing algorithms for implementation on the so-called "von Neumann" architectures - sequential machines. All the numerical analysis, data structures, efficiency, and accuracy questions studied for these architectures must now be reconsidered for architectures having anywhere from eight to many thousands of parallel processing elements. There is a clear indication that the vendor developed machines available over the next five years will consist of a few very fast vector processors. In order to use these new machines with maximum efficiency, new languages, algorithms, operating systems, and data management techniques must be devised, implemented, and tested.

The long term research questions focus on architectures that will employ a large number of processors interconnected in a variety of ways. By combining teams of mathematicians, computer scientists, computational physicists, etc., new architectures can be designed that incorporate knowledge of the entire problem and therefore provide the most effective solution. This will be a continuing basic research program, always looking for future developments in all these disciplines to lead the way to new ideas.

This is a continuing research program. No estimates for the overall costs are available as yet because the planning for the expanded long term program has just begun. We are continuing the planning exercise started by the FCCSET subcommittees to ensure that the various Federal agencies coordinate their efforts in this area.

3. **The Committee needs an explanation of the overall DOE asset management policy, program, and procedures relative to care, preservation, maintenance, upkeep, refurbishment, enhancement, and upgrade of the total DOE capital account, including physical plant, scientific equipment, supporting facilities, roads, buildings, and appurtenances thereto.**

This request is prompted by the annual DOE claim that the multiprogram general purpose facilities requests reduce the backlog of support facilities deficiencies, a claim difficult to support by the amounts involved.

Answer: The Department has established a methodology to plan for, identify, maintain, rehabilitate and construct physical plant assets necessary to perform the Department's assigned missions. Policy, guidelines, criteria are developed and maintained by the Headquarters for implementation by the field offices covering areas such as:

- Maintenance Management of Property
- Site Development and Facilities Utilization Planning
- General Design Criteria
- Construction Management
- Project Management
- Real Estate Management
- Real Property Inventory System (RPIS)

The policy of the Department is to maintain plant assets in the most economical manner commensurate with immediate program needs and the long-term interest of preserving permanent assets. Overall needs and deficiencies are reviewed and analyzed annually at Headquarters in areas such as:

- Maintenance (expense funded)
- General Plant Projects (GPP)
- General Purpose Equipment (GPE)
- Multiprogram General Purpose Facilities (MGPF)
- Specific Program related facilities projects and programs

It is not planned nor is it expected that the MGPF program will alleviate all potential deficiencies occurring at all DOE sites. As shown above there are several avenues of funding which are pursued to maintain the Department's plant assets. Each of them is reviewed and justified separately.

MGPF funding is structured to permit a phased reduction of deficiencies over the long-term in those areas eligible for MGPF funding. The program was designed to fill a gap where other programs were not adequately supporting these multi-sponsor facilities.

Necessary funding levels are also highly dependent on proper support in other areas such as expense funded maintenance and GPP. Many deficiencies can be alleviated through less expensive maintenance projects and GPP thus allowing the line-item programs such as MGPF to concentrate on rehabilitations, replacements due to obsolescence and similar requirements. Proper funding levels for these other funding areas are carefully reviewed for proper balance and support.

4. **Recently we were advised that industry participates in the DOE materials R&D program to less than 1 percent of the total program funding. Please comment.**

Answer: Industry participates to the extent of about 30% in all of the DOE materials R&D programs according to our last survey. While direct funding from the DOE Materials Sciences subprogram is less than 1 percent, it must be remembered that the Department does provide indirect support to industry in collaborative research principally at major facilities such as the National Synchrotron Light Source. This total support to industry is small because the program is one of fundamental research and most of the unsolicited proposals for this type of work come from universities. In a number of other DOE programs, for example, fossil energy, solar energy, conservation, and nuclear energy, the funding going to industry is higher than that going to universities. This is because these programs are working on applied problems, more consistent with industry's capabilities. Within DOE, the type of activity is matched with the capability of the performer.

5. **What are some examples of DOE-sponsored R&D which has found its way into industry application, excluding nuclear fission projects? What was the extent of industry involvement during the DOE sponsorship phase?**

Answer: The following are a few specific examples of BES-sponsored R&D results which have been used by industry. The typical pattern is that basic research in BES lays the foundation for new technological advances by creating a pool of knowledge. Industry can dip into this and apply it to invent radically new products or improvements to existing ones. It is important to note that DOE is very often not the sole customer for the fruits of its R&D program, and in this respect is quite different from the DOD. Therefore it is more difficult to trace the path of a development from research to product where the product development is almost entirely in the hands of the private sector. Nevertheless, we have made such a study earlier and found that significant new products and new industries have emerged from BES-sponsored research. In the following examples, as noted, there has been very little Federal support at the product development end, in most cases. Industry has found it best to fund its own product development. Additionally, it should be noted that in these situations where Federal assistance is needed for industrial developments, it is generally provided by the DOE technology programs and not the BES program. Industry, in general, has been involved in the various BES programs through participation in workshops, publications, technical meetings, review committees, attendance at DOE Laboratory information meetings and utilization of DOE facilities.

We have selected twenty examples:

a. Metallic glasses, that is non-crystalline metals, were discovered under BES contract at the California Institute of Technology. These materials are now being developed for many applications including low-loss cores for, electrical transformers and motors cores by Allied Chemical and General Electric Companies, respectively. These companies were not involved during the early BES sponsorship.

b. A process for preparing of high-purity vanadium metal by aluminothermic reduction was developed by Ames Laboratory under contract to BES. The process has been adopted commercially by Wah-Chang/Teledyne, the only domestic supplier of pure vanadium metal in quantity. There was no involvement of this company during BES sponsorship.

c. The Combustion Research Facility (CRF) was constructed with BES sponsorship and was inaugurated in 1981. Its activities are supported by

BES and other DOE elements. Already, experimental results and computer codes from the combustion research program have been used by the automotive industry to modify engine designs for greater fuel efficiency, and theoretical analyses have enabled the oil and power systems industry to devise a technique for significantly reducing a major pollutant product of combustion. At the CRF, industrial researchers are present as visiting scientists and users, as well as being active in CRF advisory activities.

d. Highly magnetostrictive alloys of terbium-dysprosium-iron were developed jointly by the Navy and Ames Laboratory, the latter under contract to BES. The alloys are useful for such applications as sonar based submarine detection, and devices are being developed by Gould, Inc., Raytheon and other industrial organizations. There was no involvement of these companies during the early DOE sponsorship but, there is now, of course, considerable involvement in prototype development.

e. Oriented graphite crystals for x-ray monochromators were developed by Oak Ridge National Laboratory for use in their BES-supported research. These crystals are now being marketed under the trade name "UCAR Oriented Graphite Crystals" by Union Carbide/Carbon Products Division. Some involvement of Union Carbide occurred during the BES sponsorship phase. The materials and design have also been exploited by Ball Bros. Research Corporation for use in x-ray polarimeters on space vehicles carrying x-ray astronomy experiments. This company was not involved during the BES sponsorship phase.

f. The economical removal of uranium (a slightly radioactive substance) during wet-process production of fertilizer from phosphate rock was made possible by the results of BES-funded research at the Oak Ridge National Laboratory on an extraction process. The simultaneous cleanup of fertilizer and production of sizable quantities of uranium makes this inexpensive process very attractive. Since 1976 five plants using it have been built by phosphate fertilizer manufacturers. Additional such plants are contemplated, for potential annual production of uranium in the range of hundreds of millions of dollars.

g. A process for making an advanced superconducting material, Nb_3Sn, was developed and patented by Brookhaven National Laboratory with support by BES. This "bronze process" has been used for about ten years by Oxford-Airco Corporation (now a division of British Oxygen Corporation) in their commerical production of multifilamentary superconducting cable for high field magnets. This company was not involved during the initial development of this process.

h. Under a BES contract scientists at Brown University formulated an effective analysis for computing the strains around a crack in the class of materials known as incompressible-fully plastic. This class is particularly complex to analyze quantitatively, and yet it is the most relevant to structures in electricity-generating energy plants. The analysis was one of the key developments enabling the Electric Power Research Institute (EPRI) to prepare its handbook, "An Engineering Approach for Elastic-Plastic Fracture Analysis"; the handbook's objective is to assist utilities in using realistic yet safe criteria in designing nuclear reactors. General Electric Corporation, an EPRI contractor, collaborated in some aspects of this research.

i. Under BES support a new method for multi-element analysis, called inductively coupled plasma atomic-emission spectroscopy, was developed at the Ames Laboratory. It is very fast, requires minute amounts of sample, and permits simultaneous identification of up to 50 elements. For most of these elements, this method is more sensitive than any other. Commercial instruments based on this development have been introduced: six U.S. and eleven foreign companies are now marketing such instruments at a sales rate of about $100 million per year.

j. Low Temperature Research at the University of California at La Jolla under a BES contract led to the development of the He^3-He^4 Dilution Refrigerator which is marketed by the Superconductivity, Helium, Electronics Corporation (S.H.E.) world-wide. Close cooperation between the university and company was maintained. S.H.E. constructed the devices.

k. IBM is conducting its own research at the National Synchrotron Light Source, BNL, in an x-ray microlithography program which is designed to enhance the corporations's capability to make important advances in dense-packed electronics including supercomputers. IBM is fully involved in the research at the NSLS and has contributed significantly to that facility's capabilities which are available to all users. The NSLS has been and continues to be operated under the aegis of BES.

l. Since 1977, a broad array of instrumentation and monitoring techniques for fossil-energy-related applications has been developed. They provide the basis for work area monitoring for industrial hygiene purposes, of a broad class of carcinogenic polyaromatic hydrocarbons (PAH) which are produced in coal conversion reactions. The instruments include the derivative ultraviolet absorption spectrometer (DUVAS) for detection of specific gaseous organic emissions, the portable "spill spotter" for detection and measurement of work surface PAH contamination, the light-pipe luminoscope for detection of PAHs on skin, and a personnel monitor for determining individual worker exposure to volatile organics, including PAHs. The capability to meet this need was a direct outgrowth of the long term support by BES of analytical research at Oak Ridge National Laboratory.

m. The combined research techniques of small angle neutron and x-ray scattering developed at Oak Ridge National Laboratory under contract to BES have led to the non-destructive testing of oil shale samples from great depth and has resulted in the determination of oil content and sizes, shapes and distribution of pores. This technique has been utilized by Chevron Petroleum Corporation. Chevron furnishes the oil shale samples; ORNL performs the scattering research.

n. Research on superconducting quantum interference devices (SQUID) at Lawrence Berkeley Laboratory, supported by BES, has led several companies to utilize the device and technique in oil and geophysical exploration including earthquake detection. No industry involvement occurred during BES sponsorship.

o. Continuous chromatography was invented by the Oak Ridge National Laboratory under BES funding. This is a promising new technique for production of purified chemicals, ranging from metal recovery to complex organics. It received an IR-100 award, has brought much interest from industrial and other organizations and has been loaned as functioning systems to industrial firms seriously considering investing in production equipment.

p. Uses of combined ion implantation and laser annealing pioneered at Oak Ridge National Laboratory with BES funding, are being employed by several industries. A young scientist now with Motorola, Inc. performed his thesis research at ORNL and is now incoporating laser techniques to improve silicon electronic devices for that company. No industry involvement occurred during the BES sponsorship phase.

q. STREM Chemicals of Newburyport, Massachusetts has acquired the process of synthesizing superconducting TMTSF organic donor material from the synthesis discovery at Argonne National Laboratory with BES support. The material is now being synthesized and sold around the world. No industry involvement occurred during DOE sponsorship phase.

r. A completely new type of rechargeable battery has been demonstrated in a laboratory model. It uses as one or both of the electrodes a conducting organic polymer, such as polyacetylene. According to the C&D Batteries Company, the conducting polymer battery "may become the most radical departure in battery making in 100 years." C&D Batteries, a subsidiary of Allied Corporation, is the largest producer of lead-acid batteries in the U.S.A. and C&D states: "the conductive polymer batteries, which are rechargeable, would have 10 times the power, one-tenth the weight and one-third the volume of conventional lead-acid batteries..." The research was performed at the University of Pennsylvania. Its initial phase was supported by the Office of Naval Research, with BES funding subsequent work aimed directly toward battery applications. The University of Pennsylvania holds a patent on the polymer battery and has licensed its development to Allied and two West German companies. There has been no industry involvement in the BES-sponsored research.

s. Helionetics, Inc. has collaborated with Oak Ridge National Laboratory, under contract to BES, in a research program involving gaseous discharge implantation and laser annealing of silicon solar cells with very high efficiences. Helionetics is utilizing the results to improve its production capability. Helionetics furnished the excimer laser necessary to the tests.

t. A vacuum distillation process was developed by Ames Laboratory for purifying calcium in order to facilitate laboratory research on rare earth preparation by metallothermic reductions. This process has been adopted by the New England Lime Company, a Division of Pfizer, Inc., and is used to prepare the major part of the calcium used in the U.S. today. The metal has important applications in steel production, metal reduction, and lead-calcium battery industries.

Materials Sciences

1. **The Narath Panel's Report on the Center for Advanced Materials, recommended that the construction of the Advanced Materials Synthesis Laboratory and the Advanced Device Concepts Laboratory be deferred until subsequent review of that plan has been completed.**

   a. How has the Department implemented this recommendation?

b. Why has the Department recommended the funding of Advanced Materials Laboratory?

Answer: a. The laboratory and DOE have decided on a limited number of topics, workshops have been held with industry participation and programs were initiated in FY 1984. The FY 1985 budget construction request includes $1.6 million for the initiation of funding for the Advanced Materials Laboratory (AML).

b. The Advanced Materials Laboratory has been reviewed by DOE and its timing is appropriate for the FY 1985 budget in view of the long lead time before the building can be occupied. The building is conventional construction and essential for the implementation of the Panel's recommendation to proceed with the materials research portion of the LBL proposal. The AML is essential for the success of the Center for Advanced Materials, and would provide needed equipment and space for the focused advanced materials research program other than surface science and catalysis. The original idea of having a separate synthesis laboratory has been modified taking into account comments and recommendations which stated that the building should await an acceptable CAM program plan. A strong effort was undertaken since the Panel report was completed to identify topics, receive industry input and review the plan and building needs.

This has been done by LBL and reviewed and approved by DOE. An Advisory Scientific Policy Board has been established, and an Interim Director, Dr. Ken Pitzer, a distinguished scientist, has been given responsibility for the evolution of the research program until a permanent Director is named. In view of the progress made to date and the long lead time before the building can be occupied, we believe this request is completely reasonable and essential in order that there be a center for advanced materials research at LBL.

2. Why, in your charge to the Narath Panel, did you not permit the Panel to consider the best location for a Materials Laboratory?

Answer: The Panel's charge was to review the LBL proposal, not to review a site for a project. In addition, the proposal was a follow up to several studies and recommendations which urged a redirection and reestablishment of DOE laboratory objectives. The LBL proposal represented a unique opportunity to address a number of Departmental objectives, and hence it was appropriate to examine the project in the light of these criteria.

3. Why has the Department recommended funding for this proposal in light of the appointment of a National Academy of Sciences Panel, under Dr. Seitz, to study all Materials Research facilities whose initial costs are $5-10 million or more?

a. Why has CAM been exempted from this scrutiny?

Answer: The Advanced Light Source (ALS) portion of the original LBL proposal (now removed) is being reviewed for priority standing by the NAS Committee. The National Academy of Sciences (NAS) Committee is reviewing major materials facilities, not buildings. The Advanced Materials Laboratory would provide needed equipment and space to house the Center for Ad vanced Materials. This building is conventional construction. The NAS Committee has the task of prioritizing major user facilities such as neutron sources and synchrotron radiation sources and perhaps other facilities such as large microscopes which are at the moment not as well defined as the neutron sources and synchroton radiation sources. CAM has been reviewed by the ad hoc technical review Panel under Dr. A. Narath. Dr. Narath is also a member of the NAS Major Materials Facilities Committee.

4. **What steps are you taking to implement the recommendations of the ERAB Report on Materials Sciences, specifically redefining the responsibilities of the energy laboratories and require all other BES materials programs, except appropriate core programs, to be competitively funded in DOE labs and universities?**

Answer: The recommendations of the ERAB Report on Materials R&D pertain to the total DOE effort in materials research, not just Materials Sciences. With regard to the recommendations specific to the Materials Sciences program, we have already underway activities which carry out the intent of the recommendations. The Materials Sciences projects at DOE Laboratories are significantly different in character than the ones at universities so that they are not in direct competition with university support. At DOE laboratories the research is facility-related, connected with the mission of the agency or of a character that requires a relatively large group of researchers working together as a team. The university projects are Professor/graduate student oriented on subjects appropriate for a thesis. We initiated this redirection several years ago. Our recent assessment of BES' university and laboratory projects affirmed to us that the quality of DOE laboratory projects is at least as good if not better than the quality of the university projects for DOE purposes. We intend to continue to fund both the DOE laboratory programs and university programs for those areas where they have expertise and special qualifications. The process is not the same, but it still involves a careful peer review process for both segments of the program.

QUESTIONS CONCERNING THE DEPARTMENT OF ENERGY'S FY 1985 SUPPORTING RESEARCH AND TECHNICAL ANALYSIS BUDGET REQUEST--SET II

GENERAL

I. BASIC ENERGY SCIENCES (BES)

1. For the period FY 1981-FY 1985, please provide, by BES subprogram, actual and estimated operating expenses, capital equipment, and construction funding.

Answer: Please see the table below for the requested information.

BASIC ENERGY SCIENCES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
NUCLEAR SCIENCES					
OPERATING EXPENSES	$ 31322	$ 35088	$ 30644	$ 37900	$ 49755
CAPITAL EQUIPMENT	830	860	1556	2150	2950
CONSTRUCTION	0	0	0	270	300
SUBPROGRAM TOTAL	32152	35948	32200	40320	53005
MATERIALS SCIENCES					
OPERATING EXPENSES	85142	93821	108163	125110	141480
CAPITAL EQUIPMENT	7100	7960	8510	12780	15450
CONSTRUCTION	625	370	2975	16440	31720
SUBPROGRAM TOTAL	92867	102151	119673	154330	188650
CHEMICAL SCIENCES					
OPERATING EXPENSES	59342	64497	70000	75500	80930
CAPITAL EQUIPMENT	4143	4930	5510	6520	8840
CONSTRUCTION	3263	325	400	450	8050
SUBPROGRAM TOTAL	66748	69752	75910	82470	97820
ENGINEERING, MATHEMATICAL AND GEOSCIENCES					
OPERATING EXPENSES	23715	24893	31050	33670	49045
CAPITAL EQUIPMENT	1764	1899	1920	2120	3000
SUBPROGRAM TOTAL	25479	26792	32970	35790	52045
ADVANCED ENERGY PROJECTS					
OPERATING EXPENSES	6314	7319	8300	9100	10810
CAPITAL EQUIPMENT	300	320	290	310	320
SUBPROGRAM TOTAL	6614	7639	8590	9410	11130
BIOLOGICAL ENERGY RESEARCH					
OPERATING EXPENSES	7237	8420	9500	10580	12490
CAPITAL EQUIPMENT	400	410	370	400	560
SUBPROGRAM TOTAL	7637	8830	9870	10980	13050
PROGRAM DIRECTION					
OPERATING EXPENSES	2104	2395	3170	3970	3830
SUBPROGRAM TOTAL	2104	2395	3170	3970	3830
BASIC ENERGY SCIENCES	**$233601**	**$253507**	**$282383**	**$337270**	**$419530**

2. For the period FY 1981 - FY 1985, please provide, by BES subprogram, actual and estimated operating expenses, capital equipment, and construction funding going to support facilities.

Answer: For consistency in definition of facilities we have provided information on 27 centers, facilities or groupings of major equipment that have been identified in Question I.C.1. These facilities fall into three categories: 1. User Facilities, 2. Imbedded Facilities -- major equipment or facilities which are part of a research program and are available on limited basis outside the funded project, and 3. Centers that are primarily operated to provide a service to the research community.

Thirteen of the facility/centers identified in the question fall into the first category. User facilities are those where facility operating support is provided separately from support for research utilization by the sponsoring DOE subprogram. In most cases, separate Field Task Proposals are submitted by the host laboratory to DOE for facility support. The following facilities fall into this category:

ANL:	High Voltage Electron Microscope Tandem Facility
	Intense Pulsed Neutron Source
BNL:	High Flux Beam Reactor
	National Synchrotron Light Source
LBL:	National Center for Electron Microscopy
LANL:	Spallation Neutron Research/Proton Storage Ring
ORNL:	High Flux Isotope Reactor
	National Center for Small Angle Scattering Research
	Oak Ridge Electron Linear Accelerator
	Shared Research Equipment Program
	Surface Modification and Characterization Laboratory
SNL-L:	Combustion Research Facility
Stanford Synchrotron Radiation Laboratory	

For each of these, a table has been prepared for insertion into the record providing the detailed information requested. For the purposes of this question, we have used the following definitions:

Operations: This includes costs to operate the facility, providing services to users, whether included under the "in-house" or "out-of-house" definitions below, and other operating expenses identified below.

In-house research: Cost of in-house user research projects, including dedicated equipment. At the IPNS, for example, the support provided by the Materials Sciences subprogram for ANL staff carrying out research using the IPNS meets this definition.

Out-of-house research: Cost to support non-host laboratory researchers using a facility, including dedicated equipment. The source of support may be DOE, other federal agencies, industry, etc. In most cases it can only be estimated although the number of outside users can normally be identified.

Other operating expenses: These include spare parts, "changes in inventory" such as for nuclear reactor fuel elements, and similar items.

Capital equipment: Includes separately budgeted equipment funds provided by BES directly to the facility.

ARIM: Includes BES provided construction funds for accelerator and reactor, improvement or modification.

GPP: Funds provided by the responsible program to the host laboratory for general plant projects which are directly related to the facility; BES does not have GPP (or GPE) budget responsibility for any of the laboratories identified in the first category except for ANL beginning in FY 1985.

In-house energy management: BES has no direct involvement in this item; any numbers provided were obtained as information from the laboratories.

(iv) Argonne National Laboratory High Voltage Electron Microscope Tandem Facility

(B/A in thousands)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	560	550	615	685	750
In-house research	BES/MS	600	750	450	500	600
	OTHER	0	0	520E	780E	860E
Out-of-house research	BES/MS*	10	10	15	20	25
	DOE, OFA INDUSTRY, OTHER	500	650	750E	800E	1200E
Capital Equipment	BES/MS	370	35	235E	900E	925E
GPP	*	0	0	0	200	800

* Numbers provided by Laboratory

E = Laboratory estimate based on number of users and time allotted

II

(v) Argonne National Laboratory Intense Pulsed Neutron Source

(B/A in thousands)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	4929	3685	3895	4712	5066
	INDUSTRY	0	0	0	17	30
In-house research	BES/MS	1410	1690	2200	2300	2400
Out-of-house research	BES/MS	N/A	0	400E	465E	540E
	DOE/OTHER	N/A	350	252E	895E	982E
	INDUSTRY	N/A	125	125E	145E	170E
	OFA/NSF	N/A	350	400E	465E	540E
	UNIV.	N/A	575	600E	700E	815E
	FOREIGN	N/A	250	400E	465E	540E
Capital Equipment	BES/MS*	180	300	300	275	450
GPP	*	12	75	70	25	145

* Numbers provided by Laboratory
E = Laboratory estimate based on number of outside users and time at IPNS

III

(viii) Brookhaven National Laboratory High Flux Beam Reactor

(B/A in thousands)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	4067	4700	6057	6600	7800
In-house research	BES/MS	2433	2630	2698	2900	3200
	BES/CS	666	722	410	420	455
	ER/NP*	962	1135	1300	826	900
	ER/BER*	528	606	624	683	727
Out-of-house research	BES/MS	0	0	307E	330E	354E
	OFA	1039	1154	1268E	1363E	1464E
	NON FED	395	438	487E	523E	563E
Other operating expenses	BES/MS	47	301	200	433	1000
Capital Equipment	BES/MS	145	175	200	400	700
	BES/CS	50	175	50	60	60
	ER/NP	181	90	90	100	125
	ER/BER	150	150	141	32	69
ARIM		0	0	0	40	500
GPP	*	0	0	66	80	120
In-house energy management	*	0	0	285	0	0

* Numbers provided by Laboratory
E = Laboratory estimate based on number of outside users and time at HFBR

IV

(ix) Brookhaven National Laboratory National Synchrotron Light Source

(B/A in thousands)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	2599	5098	5922	7795	8700
	BES/CS	0	2404	3800	4470	5600
In-house research	BES/MS	1390	1738	1604	1800	2100
	BES/CS	1009	1112	1570	1880	2030
	BES/AEP	136	165	104E	390E	90E
	ER/OTHER	0	0	493E	913E	1137E
Out-of-house research	ER/OTHER	0	0	1303E	2245E	2690E
	DOE/OTHER & OFA	1930	2315	1910E	2160E	2240E
	NON-FED	1225	1470	1980E	3225E	3960E
Other operating expenses	BES/MS	170	468	250	167	700
Capital Equipment	BES/MS	1047	1326	900	800	800
	BES/CS	288	729	770	790	340
	BES/AEP	0	0	0	160E	100E
	ER/OTHER	337	745	600E	240E	100E
ARIM		0	265	100E	600E	1100E
GPP		406	239	611E	475E	700E
In-house energy management	*	0	66	0	0	100E
Phase II construction	BES/MS	0	0	0	2500	10000

* Numbers provided by Laboratory

E = Laboratory estimate based on number of users and time allotted

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V

(xi) LBL National Center for Electron Microscopy

(B/A in thousands)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	505	767	880	1090	1490
In-house research	BES/MS	0	0	500	650	800
Out-of-house research	OTHER	0	0	500E	650E	800E
Capital Equipment		238	80	300	350	400
Other specific construction projects attributable to this facility		3152	1955	463E	270E	100E

E = Laboratory estimate based on number of outside users and time at NCEM

VI

(xii) Los Alamos National Laboratory Spallation Neutron Research/Proton Storage Ring (SNR/PSR)

(B/A in thousands)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	0	0	0	0	500
	DOE/DP*	1373	1578	1450	1600	1700
In-house research	BES/MS	819	1190	1530	1570	1800
	DOE/DP*	600	635	710	800	1165
Capital Equipment	BES/MS	130	250	250	300	600
	OTHER*	13	50	50	90	100
GPP	*	390	0	0	0	0
SNR Improvement project	BES/MS	0	0	2700	0	0

* Numbers provided by Laboratory

VII

(xviii) ORNL High Flux Isotope Reactor

(B/A in thousands)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/NS	3494	3798	5590	6150	7820
	BES/MS	781	918	0	0	0
	DOE/NE	182	130	100	0	0
	ER/OFE	146	400	0	0	0
	ER/HER	182	200	0	0	0
(Rev. fm isotope sales)		779	842	644	805	726
(Rev. fm other, internal sources/services provided:		198	311	383	409	355
In-house research	BES/MS	1894	1602	1868E	2190E	2370E
	ER/OFE	1200	1350	1460E	1617E	1545E
	DOE/NE	800	650	583E	500E	600E
Out-of-house research	DOE, OFA, INDUSTRY, OTHER	600	700	950E	720E	1540E
	RES EQ*	0	0	679E	720E	0E
Other operating expenses	BES/NS	0	0	0	0	1450
Capital Equipment	BES/MS	82	170	200	400	600
	BES/NS	152	484	70	120	80
ARIM		0	0	0	0	300E
GPP		0	0	0	0	250E

* Includes specialized research equipment for use at HFIR and Japanese neutron diffractometer

E = Laboratory estimate based on number of outside users and time at HFIR

VIII

(xix) ORNL National Center for Small-Angle Scattering Research
(Center dependent on neutrons produced at HFIR)

(B/A in thousands)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	NSF*	463	486	472	466	625
In-house research	NSF*	88	95	91	89	142
	BES/MS*	100	100	90	90	100
Out-of-house research	DOE, OFA, OTHERS	1200	1200	800E	800E	1200E
Capital Equipment	NSF*	0	0	60	100	26
Other Construction		0	124	0	0	0

* Estimate by Laboratory of sources of in house support from various projects

E = Laboratory estimate based on number of outside users and time using small angle scattering facility

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IX

(xx) Oak Ridge Electron Linear Accelerator (ORELA)

(B/A in thousands)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/NS	1261	1443	1546	1600	1650
In-house research	BES/NS	947	1185	1363	1520	1765
	HENP/NP	609	553	50	50	50*
	OFA	28	27	37	38	32
	ER/OTHER	0	31	36	40	43
	DOE/NE	1008	980	856	756	200
Capital Equipment	BES/NS	153	154	154	180	500
	HENP/NP	99	107	0	0	0
	DOE/NE	57	67	17	0	0
GPP	*	0	0	340	0	0

* Decrease because of reprogramming of funds to Holifield Facility

X

(xxi) ORNL Shared Research Equipment Program (SHaRE)

(B/A in thousands)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	220	230	260	290	320
	BES/OTHER	40	45	50	55	58
In-house research *	BES/MS	900	1000	1292E	1680E	1930E
	ER/MFE	190	200	200E	220E	250E
	CONS	0	0	75E	80E	85E
	FOSSIL	20	30	50E	60E	70E
	NUCLEAR	200	150	100E	50E	50E
Out-of-house research	DOE, OFA, INDUSTRY, OTHER	810	1032	1047E	1137E	1195E
Capital Equipment	BES/MS	25	370	75E	290E	325E
	ER/FE	0	250	325E	0	0
	DOE/NE	0	50	0	0	0
ARIM		0	0	325E	0	0

* Estimate by Laboratory of sources of in-house support from various projects
E = Laboratory estimate based on number of users and equipment used

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XI

(xxii) ORNL Surface Modification and Characterization Laboratory

(B/A in thousands)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	0	0	460	500	850
In-house research	BES/MS	857	1283	1120	1220	1280
	ER/OFE	125E	195E	125E	125E	125E
	OTHER	0	0	50	0	0
Out-of-house research	DOE, OFA, INDUSTRY, OTHER	0	0	400E	400E	600E
Other Operating Expenses		70	0	0	200E	0
Capital Equipment		99	633	257E	595E	825E
GPP		0	235E	235E	650E	500E

E = Laboratory estimate based on number of outside users and time at SMCL

XII

(xxv) Sandia National Laboratories Combustion Research Facility

(B/A In thousands)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/CS	1900	1930	2170	2490	2750
In-house research	BES/CS	1400	1840	2160	2290	2500
	BES/OTHER*	870	1020	1340	1450	1560
	DP*	0	0	500	750	1000
	CE*	1200	1350	1450	1650	1900
	OFA/NRC*	0	0	330	500	670
	FOSSIL*	1030	1650	1320	1400	1700
Out-of-house research	BES/CS*	300	480	680	730	770
	INDUSTRY	0	0	40E	20E	200E
Capital Equipment		800	975	900	800	700
GPP		0	0	0	100	530

* Numbers provided by Laboratory
E = Laboratory estimate based on number of outside users and time at CRF

XIII

(xxvi) Stanford Synchrotron Radiation Laboratory

(B/A In thousands)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations**	BES/NS	***	***	6192	6577	7980
In-house research	BES/NS	0	0	152	159	0
	BES/MS	0	0	0	700	895
Out-of-house research	BES/NS	0	0	0	0	0
	OTHER*	0	0	21600E	3200E	42900E
Capital Equipment	BES/NS	0	0	456	490	600
	BES/MS	0	0	0	100	300
GPP		0	0	0	0	100
Other specific construction projects attributable to this facility		0	0	100E	2790E	1,0130E

* Numbers provided by Laboratory
** Operated primarily as a user facility
*** Funded by NSF in 1981 and 1982

E = Laboratory estimate based on number of outside users, time on SSRL and time at home institutions devoted to preparing experiments, analyzing data

Eight of the facility/centers fall into the second category of "Imbedded Facilities". They involve specialized pieces of equipment which are central to, and part of, the conduct of a large research project. Their operating costs are usually not separately broken out but are included in the funds provided for the implementation of the research project employing them. The equipment/facility may be made available to qualified users on a case-by-case basis at no cost, when appropriate. The imbedded facility/centers are:

ANL Atomic Spectroscopy Facility
ANL 4.5-MV Dynamitron Accelerator
ANL Pulse Radiolysis Facility
Kansas State University James R. Macdonald Laboratory
Notre Dame Radiation Laboratory Pulse Radiolysis Facility
Notre Dame Radiation Laboratory Radiolysis ESR Facility
ORNL EN-Tandem Facility
Research Computer Facilities

The ANL 4.5 MV Dynamitron and the ANL Pulse Radiolysis Facilities are jointly funded by BES and HENP. Accelerator and Reactor Improvement and Modification funds have been provided to these facilities as follows:

	(B/A in thousands)				
	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
ANL 4.5 MV Dynamitron (Nuc. Physics)	0	0	300	100	0
ORNL EN-Tandem Facility	200	0	100	250	0

The Kansas State University James R. Macdonald Laboratory is a university-owned atomic physics facility. Research support provided by BES includes funding for operation of an accelerator. Included in the BES FY 1985 request are funds, $2 million, to initiate upgrading of the accelerator at a total estimated cost of $3.4 million to DOE ($1.4 million will be requested to complete the project in FY 1986). Additionally, the State of Kansas will provide $0.6 million to upgrade the housing for the accelerator.

There are 11 Research Computer Facilities, 10 at DOE laboratories and 1 at a university, each consisting of one or more minicomputers dedicated primarily to a specific thrust of the Applied Mathematical Sciences subprogram of BES. Operation of the facilities is supported within the framework of each of the individual projects. Capital equipment funding for these facilities was $800 thousand in FY 1983, $970 thousand in FY 1984, and the FY 1985 request is for $1.5 million.

Five of the facility/centers fall into the third category. Service facilities generally do not have a research component directly at the facility except to improve the service provided, and operate on a subsidized or cost reimbursable basis. They are listed below and discussed separately.

Ames Laboratory Materials Preparation Center
ANL Premium Coal Sample Bank
LANL Equation of State Library
ORNL Electromagnetic Isotope Preparation Program
ORNL Transuranium Processing Plant

Ames Laboratory Materials Preparation Center

$K

	Budget Authority			
	FY 1982	FY 1983	FY 1984	FY 1985
Operations - Total	366	892	950	1067
Ames Laboratory Orders	216	687	740	817
Non Ames Laboratory Orders	150	205	210	250

The facility started operating in FY 1982. It operates on a cost reimbursable basis and has no independent facility operating budget. The center consists of special sample preparation apparatus and personnel trained in its use. Samples which are not available from other sources are prepared on order according to specifications on a best effort basis. The center also provides analytical services and acts as a clearing house/referral system for information about the availability of special research samples.

ANL Premium Coal Sample Program

$K

	Budget Authority		
	FY 1983	FY 1984	FY 1985
Operating - Chemical Sciences	454	645	622

Funding for the ANL Premium Coal Sample Program was first provided in FY 1983. This program collects, prepares and distributes reference grade samples of a small number of representative coals for the use of qualified researchers to establish benchmark experimental measurements in coal science. Exceptionally uniform samples are specially prepared and stored in an inert atmosphere to ensure the chemical stability of the coal over a long period of time.

Los Alamos Equation of State Library

$K

	Budget Authority				
	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operating total	0	0	320	350	250
Operating BES - Materials Sciences	140	125	120	125	0
Other - Defense Programs	160	180	200	225	250(Est.)

This facility is a computer based Library of Equation of State data and FORTRAN subroutines developed at Los Alamos which are made available without charge to qualified scientists and engineers.

ORNL Electromagnetic Isotope Preparation Facility
$K

	Budget Authority				
	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operating total	2400	3615	3263	3580	5000
Facility	2180	3379	3013	3220	4630
R&D	220	236	250	360	370
Operating Source	2400	3615	3275	3580	5000
Isotope Sales	1380	2860	2205	2500	2700
OHER	0	0	250	400	600
BES - Nuclear Science	1020	755	820	680	1700
Capital Equipment					
BES - Nuclear Science	48	32	200	500	500
ARIM	0	0	0	270	0
GPP	0	0	0	0	100

This facility separates stable isotopes for the Research Materials Collection (non consumable).

ORNL Transuranium Processing Plant (TRU)
$K

	Budget Authority				
	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operating total	4953	5554	6173	6473	6799
Separations BES - Nuc. Sci.	3740	4200	4800	5136	5490
Process R&D (NE)	1095	1175	1148	1157	1167
Misc. Reimbursable Services	75	92	134	85	92
Capital Equipment BES - Nuc. Sci.	43	52	91	95	50
Nuclear Energy	0	35	0	0	0

This facility is used to perform two functions. Its principal use is the chemical separation of heavily irradiated target materials for the purpose of preparing research samples of the rare, highly radioactive transuranium elements, none of which occur in nature. A secondary effort is devoted to chemical separations process development funded by the Nuclear Energy program.

3. For the period FY 1981 - FY 1985, please provide, by BES subprogram and by DOE laboratory, actual and estimated BES funding going to DOE laboratories.

Answer: Please see the table below for the requested information.

BASIC ENERGY SCIENCES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
NUCLEAR SCIENCES					
OPERATING EXPENSES					
AMES LAB	$ 200	$ 185	$ 0	$ 0	$ 0
ARGONNE NATIONAL LAB	3055	3295	1237	1300	1820
BROOKHAVEN NATIONAL LAB	4527	5323	1910	2057	2800
IDAHO NATIONAL ENG LAB	265	320	290	300	520
LAWRENCE BERKELEY LAB	2447	2445	1504	5135	6115
LAWRENCE LIVERMORE NAT LAB	470	437	265	210	220
LOS ALAMOS NATIONAL LAB	1295	1415	1288	2300	3075
MOUND LABORATORY	111	149	157	140	232
OAK RIDGE NATIONAL LAB	12028	13755	15695	16671	21610
PACIFIC NORTHWEST LABS	250	200	244	250	260
SANDIA CORP	25	0	0	0	0
STANFORD UNIVERSITY-SLAC	0	0	0	50	50
CAPITAL EQUIPMENT					
ARGONNE NATIONAL LAB	101	90	100	100	100
BROOKHAVEN NATIONAL LAB	32	40	40	50	50
IDAHO NATIONAL ENG LAB	25	25	25	25	25
LAWRENCE BERKELEY LAB	80	85	90	265	590
LAWRENCE LIVERMORE NAT LAB	5	0	0	0	0
LOS ALAMOS NATIONAL LAB	89	83	140	145	225
OAK RIDGE NATIONAL LAB	450	472	645	950	1240
PACIFIC NORTHWEST LABS	23	20	20	20	20
CONSTRUCTION					
OAK RIDGE NATIONAL LAB	0	0	0	270	300

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
MATERIALS SCIENCES					
OPERATING EXPENSES					
AMES LAB	6010	6720	7160	7520	7900
ARGONNE NATIONAL LAB	17320	18398	19990	21000	22260
BROOKHAVEN NATIONAL LAB	11080	14468	20730	23370	27600
IDAHO NATIONAL ENG LAB	470	370	400	550	580
LAWRENCE BERKELEY LAB	5580	6490	7800	13300	15300
LAWRENCE LIVERMORE NAT LAB	1190	1260	1584	1520	1770
LOS ALAMOS NATIONAL LAB	2650	3080	3727	3900	4500
MOUND LABORATORY	250	120	0	0	0
OAK RIDGE NATIONAL LAB	16370	18528	19038	21030	23200
PACIFIC,NORTHWEST LABS	1880	1880	1960	2050	2070
SANDIA CORP	2138	2260	2360	3120	3400
SANDIA LAB, LIVERMORE	500	600	910	980	1050
SERI	260	270	350	420	450
CAPITAL EQUIPMENT					
AMES LAB	730	730	810	750	800
ARGONNE NATIONAL LAB	1640	1480	1670	2220	2700
BROOKHAVEN NATIONAL LAB	1540	1950	1900	1240	1800
IDAHO NATIONAL ENG LAB	60	30	40	170	60
LAWRENCE BERKELEY LAB	540	660	790	2670	2200
LAWRENCE LIVERMORE NAT LAB	90	50	100	150	200
LOS ALAMOS NATIONAL LAB	300	350	600	900	800
MOUND LABORATORY	20	0	0	0	0
OAK RIDGE NATIONAL LAB	1710	2100	2090	2700	2900
PACIFIC NORTHWEST LABS	170	170	180	200	250
SANDIA CORP	180	220	200	290	340
SANDIA LAB, LIVERMORE	100	200	100	140	150
SERI	20	20	30	50	100
CONSTRUCTION					
AMES LAB	275	275	275	275	600
BROOKHAVEN NATIONAL LAB	350	95	0	3140	11100
LAWRENCE BERKELEY LAB	0	0	0	2060	12290
LOS ALAMOS NATIONAL LAB	0	0	2700	0	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
CHEMICAL SCIENCES					
OPERATING EXPENSES					
AMES LAB	2408	2665	2812	2946	3130
ARGONNE NATIONAL LAB	8029	9320	10612	11347	11766
BARTLESVILLE EN TECH CTR	160	153	149	177	186
BROOKHAVEN NATIONAL LAB	9418	12395	12555	13767	14989
IDAHO NATIONAL ENG LAB	100	120	165	120	126
LAWRENCE BERKELEY LAB	4405	5415	6299	6214	6125
LAWRENCE LIVERMORE NAT LAB	310	240	235	30	45
LOS ALAMOS NATIONAL LAB	715	870	715	719	504
MOUND LABORATORY	950	916	978	950	730
OAK RIDGE NATIONAL LAB	7010	7420	7725	7716	7931
PACIFIC NORTHWEST LABS	1235	1128	1300	1310	1414
PITTSBURGH ENER TECH CTR	61	95	78	93	87
SANDIA CORP	245	310	410	655	533
SANDIA LAB, LIVERMORE	4150	4445	5010	5509	6000
SERI	370	530	600	731	839
CAPITAL EQUIPMENT					
AMES LAB	315	403	335	447	450
ARGONNE NATIONAL LAB	750	880	885	1105	3475
BARTLESVILLE EN TECH CTR	10	0	20	15	22
BROOKHAVEN NATIONAL LAB	904	1122	1376	1491	1303
IDAHO NATIONAL ENG LAB	5	10	12	11	15
LAWRENCE BERKELEY LAB	370	470	918	1071	731
LAWRENCE LIVERMORE NAT LAB	25	15	13	3	5
LOS ALAMOS NATIONAL LAB	55	60	52	64	60
MOUND LABORATORY	65	60	71	71	81
OAK RIDGE NATIONAL LAB	535	510	562	691	846
PACIFIC NORTHWEST LABS	85	75	90	116	169
PITTSBURGH ENER TECH CTR	5	5	5	7	10
SANDIA CORP	10	20	29	58	64
SANDIA LAB, LIVERMORE	800	975	905	800	700
SERI	20	35	44	65	100
CONSTRUCTION					
ARGONNE NATIONAL LAB	0	0	300	100	5200
BROOKHAVEN NATIONAL LAB	0	300	75	0	600
LAWRENCE BERKELEY LAB	3000	0	0	0	0
OAK RIDGE NATIONAL LAB	200	0	0	250	200
SANDIA LAB, LIVERMORE	38	0	0	100	0

ENGINEERING, MATHEMATICAL AND GEOSCIENCES

OPERATING EXPENSES

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
AMES LAB	325	400	500	600	725
ARGONNE NATIONAL LAB	2030	2185	2430	2680	3213
BROOKHAVEN NATIONAL LAB	400	425	600	630	675
IDAHO NATIONAL ENG LAB	130	150	200	275	295
LAWRENCE BERKELEY LAB	2585	2755	3185	3059	3181
LAWRENCE LIVERMORE LAB	1790	1467	2280	2700	2668
LOS ALAMOS NATIONAL LAB	2188	2275	2789	3590	2950
OAK RIDGE NATIONAL LAB	1120	1130	1380	1690	1856
PACIFIC NORTHWEST LABS	1240	1170	1153	1205	1089
SANDIA CORP	1475	1771	1982	2260	2352
SANDIA LAB, LIVERMORE	425	450	550	595	645

CAPITAL EQUIPMENT

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
AMES LAB	88	20	50	95	20
ARGONNE NATIONAL LAB	142	155	190	180	30
IDAHO NATIONAL ENG LAB	54	0	40	20	20
LAWRENCE BERKELEY LAB	285	225	610	280	120
LAWRENCE LIVERMORE NAT LAB	113	370	200	180	120
LOS ALAMOS NATIONAL LAB	265	205	180	170	150
OAK RIDGE NATIONAL LAB	196	285	135	190	290
PACIFIC NORTHWEST LABS	116	55	55	110	70
SANDIA CORP	252	190	100	120	130
SANDIA LAB, LIVERMORE	0	30	0	0	0

ADVANCED ENERGY PROJECTS

OPERATING EXPENSES

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
ARGONNE NATIONAL LAB	0	0	512	600	700
BRUOKHAVEN NATIONAL LAB	406	859	30	662	520
FERMILAB	10	0	- 8	0	0
IDAHO NATIONAL ENG LAB	0	132	694	240	600
LAWRENCE BERKELEY LAB	0	620	400	500	700
LAWRENCE LIVERMORE NAT LAB	50	360	204	150	460
LOS ALAMOS NATIONAL LAB	0	333	1168	819	900
PRINCETON PLASMA PHYS LAB	251	266	305	110	300
SANDIA CORP	223	392	110	201	200
SERI	185	128	143	18	300

CAPITAL EQUIPMENT

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
BROOKHAVEN NATIONAL LAB	180	158	106	138	100
LAWRENCE BERKELEY LAB	0	10	10	0	0
LAWRENCE LIVERMORE NAT LAB	0	0	30	50	100
LOS ALAMOS NATIONAL LAB	0	12	94	50	100
PRINCETON PLASMA PHYS LAB	51	50	20	0	20
SANDIA CORP	0	50	30	10	0
SERI	35	0	0	0	0

BIOLOGICAL ENERGY RESEARCH

OPERATING EXPENSES					
BROOKHAVEN NATIONAL LAB	830	850	915	980	1200
LAWRENCE BERKELEY LAB	790	840	910	1011	1200
LAWRENCE LIVERMORE NAT LAB	0	0	20	0	0
LOS ALAMOS NATIONAL LAB	0	0	0	0	200
OAK RIDGE NATIONAL LAB	0	150	200	200	200
SERI	100	100	105	105	120
CAPITAL EQUIPMENT					
BROOKHAVEN NATIONAL LAB	25	25	70	50	50
LAWRENCE BERKELEY LAB	50	60	50	50	50

4. **For the period FY 1981 - FY 1985, please provide, by BES subprogram and by university, actual and estimated BES funding going to university researchers.**

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
NUCLEAR SCIENCES					
OPERATING EXPENSES					
CLARK UNIVERSITY	$ 58	$ 58	$ 0	$ 0	$ 0
COLORADO SCHOOL MINES	0	0	47	75	60
COLORADO UNIV OF	719	400	0	0	0
CORNELL UNIV	67	55	0	0	0
DENISON UNIVERSITY	28	34	49	49	40
DUKE UNIV	980	1265	0	0	0
FLORIDA STATE UNIV	77	85	89	96	102
GEORGIA INS OF TECHNOLOGY	43	43	0	0	0
INDIANA UNIV	- 1	0	0	0	0
IOWA STATE UNIV - AMES	110	0	0	0	0
KENTUCKY UNIV OF	60	0	0	0	0
LOWELL UNIV OF	92	116	120	124	130
MAINE UNIV OF	0	- 11	0	0	0
MARYLAND UNIV OF	65	79	0	0	0
MASSACHUSETTS INST TECH	20	- 40	0	0	0
MICHIGAN UNIV OF	130	153	158	170	180
MIDDLE TENNESSEE STATE	35	32	0	36	40
NEW MEXICO UNIV OF	42	115	180	129	138
NEW YORK CITY U - BROOKLYN	142	153	0	0	0
NEW YORK ST UNIV OF ALBANY	38	39	41	0	0
NORTH CAROLINA STATE U	145	175	80	50	55
NORTH CAROLINA UNIV OF	170	191	0	0	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
NORTH TEXAS STATE UNIV	0	8	0	0	0
OHIO UNIV	150	195	215	235	250
OKLAHOMA UNIV OF	0	45	0	0	0
OREGON STATE UNIV	0	0	30	0	0
PENNSYLVANIA UNIV OF	89	89	96	92	95
STANFORD UNIVERSITY-SSRL	0	100	5894	6736	7880
TENNESSEE TECH UNIV	0	66	0	0	0
TENNESSEE UNIV OF	202	219	224	235	268
TEXAS A & M UNIV	460	600	0	0	0
WASHINGTON UNIV OF	735	1339	0	0	0
WISCONSIN UNIV OF	723	514	0	0	0
YALE UNIV	500	659	0	0	0
CAPITAL EQUIPMENT					
STANFORD UNIVERSITY-SSRL	0	0	456	490	600
MATERIALS SCIENCES					
OPERATING EXPENSES					
ARIZONA STATE UNIV	80	165	182	200	232
ARIZONA UNIV OF	0	0	72	75	82
BOSTON UNIV	52	71	162	0	0
BRANDEIS UNIV	0	0	44	0	45
BROWN UNIV	238	260	362	305	429
CALIF UNIV OF DAVIS	145	139	237	223	210
CALIF UNIV OF IRVINE	191	192	222	214	268
CALIF UNIV OF LOS ANGELES	93	90	61	0	0
CALIF UNIV OF SAN DIEGO	335	379	399	438	465
CALIF UNIV OF SANTA BARBARA	154	85	244	99	207
CALIFORNIA INST OF TECH	322	316	302	363	387
CARNEGIE MELLON UNIV	122	64	148	75	120
CASE WESTERN RESERVE U	387	259	201	0	178
CATHOLIC UNIV OF AMERICA	57	4	0	0	0
CHICAGO UNIV OF	116	118	138	140	157
CLARK COLLEGE	0	0	70	0	85
COLORADO RESEARCH INST	0	0	0	67	71
COLORADO SCHOOL MINES	135	145	152	156	185
COLORADO UNIV OF	0	90	187	110	120
COLUMBIA UNIV	56	67	79	87	110
CONNECTICUT UNIV OF	195	320	266	150	151
CURNELL UNIV	1076	828	761	1039	805
DARTMOUTH COLLEGE	163	66	88	97	125
DELAWARE UNIV OF	112	125	60	73	80
DENVER UNIV OF	147	77	153	152	160
EMORY UNIV	86	83	44	0	0
FLORIDA STATE UNIV	55	56	102	0	0
FLORIDA UNIV OF	200	120	266	105	573
FRANKLIN INSTITUTE	0	22	24	25	27
GEORGIA INS OF TECHNOLOGY	175	140	149	159	172

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
HARVARD UNIV	0	90	373	120	345
HOUSTON UNIV OF	77	74	0	0	0
ILLINOIS INST TECH	112	0	- 2	0	0
ILLINOIS UNIV OF	2640	3046	3038	3222	3535
INDIANA UNIV	5	0	0	0	0
JOHNS HOPKINS UNIV	63	70	0	0	0
KENTUCKY UNIV UF	137	238	189	264	301
LEHIGH UNIV	205	154	314	76	397
LOUISIANA STATE UNIV	56	58	62	65	76
MARYLAND UNIV OF	146	155	175	195	210
MASSACHUSETTS INST TECH	1606	1741	2125	1713	2382
MASSACHUSETTS UNIV OF	90	74	85	105	0
MICHIGAN STATE UNIV	55	54	61	61	0
MICHIGAN TECH UNIV	75	118	0	94	105
MICHIGAN UNIV OF	126	210	129	251	275
MINNESOTA UNIV OF	1231	1148	1099	1521	1100
MISSOURI UNIV OF	128	145	327	180	180
NEVADA UNIV OF	0	0	78	0	0
NEW MEX INST MING TECHNL	58	90	95	0	0
NEW MEXICO UNIV OF	0	0	95	0	0
NEW YORK CITY U - BROOKLYN	0	79	164	90	0
NEW YORK CITY U - CITY CL	228	150	127	91	98
NEW YORK ST UNIV OF ALBANY	0	0	5	0	0
NEW YORK ST U OF ST BROOKE	622	759	850	1081	1480
NORTH CAROLINA A&T STATE U	0	0	50	0	75
NORTH CAROLINA STATE U	0	335	365	240	385
NORTH CAROLINA UNIV OF	59	38	0	0	0
NORTHEASTERN UNIV	98	89	79	100	0
NORTHWESTERN UNIV	446	302	507	210	230
NOTRE DAME UNIV OF	141	0	90	85	75
OAK RIDGE ASSOC UNIV	105	130	140	170	200
OHIO STATE UNIV	200	232	244	370	460
OREGON STATE UNIV	74	50	69	85	90
OREGON UNIV OF	- 32	0	0	0	0
PENNSYLVANIA STATE UNIV	342	413	454	419	696
PENNSYLVANIA UNIV OF	400	434	372	291	394
PITTSBURGH UNIV OF	61	61	65	71	75
POLYTECHNIC INST BKLYN	60	65	75	90	95
PRINCETON UNIV	120	0	73	0	88
PURDUE UNIV	239	697	760	758	903
RENSSELAER POLYTECHNIC	431	580	506	593	405
RICE WILLIAM MARSH UNIV	157	194	230	240	285
ROCHESTER UNIVERSITY OF	161	172	187	181	95
RUTGERS UNIV	0	151	189	200	230
SERI UNIVERSITY PGM	500	0	0	0	0
SOUTHERN CAL UNIV OF	180	235	251	194	260
SOUTHERN ILL UNIVERSITY	70	73	77	93	100
STANFORD LELAND JR UNVR	674	462	662	589	830
STANFORD UNIVERSITY-SSRL	0	0	0	700	1700
STEVENS INST OF TECH	180	65	84	130	104
SYRACUSE UNIV	92	80	119	0	180
TENNESSEE UNIV OF	187	134	0	140	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
TEXAS UNIV OF	105	87	88	115	125
UTAH UNIV OF	200	220	137	177	289
VIRGINIA POLYTECHNIC INST	113	144	25	77	87
VIRGINIA UNIV OF	152	165	237	197	253
WASHINGTON UNIV OF	122	225	159	180	301
WASHINGTON UNIV ST LOUIS	200	0	0	0	0
WEST VIRGINIA UNIV	0	0	57	0	65
WISCONSIN UNIV OF	172	199	313	364	371
CAPITAL EQUIPMENT					
STANFORD UNIVERSITY-SSRL	0	0	0	100	300
CONSTRUCTION					
CATHOLIC UNIV OF AMERICA	0	0	0	5000	0
COLUMBIA UNIV	0	0	0	5000	0
NOTRE DAME UNIV OF	0	0	0	25	0
STANFORD UNIVERSITY-SSRL	0	0	0	940	7730
CHEMICAL SCIENCES					
OPERATING EXPENSES					
ALABAMA A&M UNIV	0	0	0	100	0
ALABAMA UNIV OF	53	58	63	67	71
AMHERST COLLEGE	41	47	47	49	50
ARIZONA UNIV OF	188	202	270	159	254
ARKANSAS UNIV OF	37	40	0	42	48
BOSTON UNIV	368	88	435	75	272
BRANDEIS UNIV	80	96	90	95	100
BRIGHAM YOUNG UNIV	212	194	251	213	228
BROWN UNIV	147	167	183	209	221
CALIF UNIV OF BERKELEY	80	88	0	80	0
CALIF UNIV OF DAVIS	129	205	48	82	85
CALIF UNIV OF IRVINE	294	275	311	333	350
CALIF UNIV OF LOS ANGELES	266	333	287	300	310
CALIF UNIV OF SAN DIEGO	0	55	61	64	0
CALIF UNIV OF SANTA BARBARA	316	359	265	257	305
CALIFORNIA INST OF TECH	271	400	268	395	418
CARNEGIE MELLON UNIV	0	60	60	50	0
CHICAGO UNIV OF	275	275	310	373	309
CLARKSON COLLEGE OF TECH	0	60	68	155	0
CLEMSON UNIV	0	110	0	65	0
COLORADO STATE UNIV	112	52	125	138	145
COLORADO UNIV OF	295	415	264	402	422
COLUMBIA UNIV	134	358	182	410	234
CONNECTICUT UNIV OF	3	0	51	54	56
CORNELL UNIV	224	300	292	294	295
DARTMOUTH COLLEGE	0	0	82	0	41
DREXEL UNIVERSITY	110	0	55	60	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
FLORIDA STATE UNIV	42	0	0	0	0
FLORIDA UNIV OF	56	60	69	71	75
GEORGE WASHINGTON UNIV	0	0	0	58	70
GEORGIA INS OF TECHNOLOGY	54	55	60	66	70
GEORGIA UNIV OF	139	168	125	209	208
HARVARD UNIV	126	90	95	100	108
HEBREW UNIV	11	0	0	0	0
HOUSTON UNIV OF	145	320	164	258	269
HOWARD UNIV	47	47	45	55	56
ILLINOIS INST TECH	190	136	166	177	190
ILLINOIS UNIV OF	151	160	165	301	190
INDIANA UNIV	230	44	262	54	209
JACKSON STATE UNIV	0	0	50	55	60
JOHNS HOPKINS UNIV	232	56	146	143	152
KANSAS STATE UNIV	543	634	625	676	734
KANSAS UNIVERSITY OF	124	130	144	154	166
KENT STATE UNIV	54	60	57	66	0
KENTUCKY UNIV OF	185	48	70	0	0
LEHIGH UNIV	0	0	297	86	115
LOUISIANA STATE UNIV	132	25	70	117	123
MARQUETTE UNIV	44	105	0	60	63
MARYLAND UNIV OF	95	108	107	0	0
MASSACHUSETTS INST TECH	300	406	724	435	609
MASSACHUSETTS UNIV OF	186	0	126	0	76
MINNESOTA UNIV OF	583	519	484	465	389
MISSOURI UNIV OF	69	68	129	137	149
MOREHOUSE COLLEGE	0	0	44	48	0
MOUNT HOLYOKE COLLEGE	56	114	0	65	0
NEBRASKA UNIV OF	248	230	199	283	230
NEW MEXICO UNIV OF	88	97	90	105	110
NEW ORLEANS UNIV OF	50	47	55	60	64
NEW YORK CITY U - BROOKLYN	0	0	-5	0	0
NEW YORK CITY U - NEW YORK	0	0	80	80	60
NEW YORK ST U OF BUFFALO	60	57	62	64	68
NEW YORK ST U OF ST BROOKE	464	312	396	211	330
NEW YORK UNIV	80	0	80	90	90
NORTH CAROLINA STATE U	64	0	0	0	0
NORTH CAROLINA UNIV OF	335	212	305	329	355
NORTHWESTERN UNIV	280	318	155	338	347
NOTRE DAME UNIV OF	2232	2450	2663	2835	3005
OHIO STATE UNIV	278	134	140	104	0
OKLAHOMA UNIV OF	100	86	86	65	63
OREGON GRADUATE CENTER	0	0	90	0	70
OREGON STATE UNIV	45	45	0	0	0
OREGON UNIV OF	45	7	29	0	0
PENNSYLVANIA STATE UNIV	390	349	410	486	451
PENNSYLVANIA UNIV OF	0	0	84	169	179
PITTSBURGH UNIV OF	125	179	234	221	226
PRINCETON UNIV	208	78	282	309	335
PUERTO RICO UNIV OF	0	45	125	0	0
PURDUE UNIV	338	217	283	300	331
RENSSELAER POLYTECHNIC	0	83	265	85	185

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
RICE WILLIAM MARSH UNIV	279	298	356	458	275
ROCHESTER UNIVERSITY OF	109	116	185	396	222
RUTGERS UNIV	84	63	5	0	0
SAN DIEGO ST UNIV FDT	0	0	60	65	68
SERI UNIVERSITY PGM	500	0	0	0	0
SOUTHERN CAL UNIV OF	60	60	0	0	0
ST JOHN FISHER COLLEGE	0	109	0	60	0
STANFORD LELAND JR UNVR	583	470	402	588	443
SYRACUSE UNIV	164	164	241	324	328
TEMPLE UNIV	130	0	67	80	0
TENNESSEE UNIV OF	130	135	241	250	256
TEXAS A & M UNIV	415	253	289	226	240
TEXAS SOUTHERN UNIV	46	27	0	0	0
TEXAS TECH UNIV	43	43	112	91	125
TEXAS UNIV OF	250	130	123	197	137
TOLEDO UNIV OF	0	21	55	0	32
UTAH UNIV OF	290	465	379	523	366
VANDERBILT UNIV	59	72	78	82	88
VERMONT UNIV OF	46	0	0	0	0
VIRGINIA UNIV OF	59	63	73	64	67
WASHINGTON STATE UNIV	60	60	0	75	0
WASHINGTON UNIV OF	0	0	0	70	75
WASHINGTON UNIV ST LOUIS	81	85	86	93	90
WAYNE STATE UNIV	149	207	160	160	68
WEBER STATE COLLEGE	55	45	0	0	0
WESLEYAN UNIV	115	0	- 45	0	0
WESTERN MICHIGAN UNIV	0	0	37	55	65
WILLIAM & MARY COLL OF	65	72	75	80	85
WISCONSIN UNIV OF	130	191	22	191	171
WORCESTER POLYTECH INST	78	0	43	0	0
WRIGHT STATE UNIV	135	138	55	59	65
WYOMING UNIV OF	63	67	77	77	81
YALE UNIV	359	274	248	378	408
CAPITAL EQUIPMENT					
NOTRE DAME UNIV OF	190	290	193	252	359
CONSTRUCTION					
KANSAS STATE UNIV	0	0	0	0	2000
NOTRE DAME UNIV OF	25	25	25	0	50
ENGINEERING, MATHEMATICAL AND GEOSCIENCES					
OPERATING EXPENSES					
ALASKA UNIV OF	178	113	109	120	129
ARIZONA STATE UNIV	62	66	123	0	62

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
ARIZONA UNIV OF	166	158	149	110	114
ATLANTA UNIVERSITY	0	0	62	67	70
BRIGHAM YOUNG UNIV	0	0	0	20	60
BROWN UNIV	265	261	493	140	281
CALIF UNIV OF BERKELEY	394	482	731	293	385
CALIF UNIV OF LOS ANGELES	417	180	121	192	72
CALIF UNIV OF SAN DIEGO	0	0	0	50	0
CALIF UNIV OF SANTA BARBARA	0	0	0	40	0
CALIFORNIA INST OF TECH	163	163	871	939	1553
CARNEGIE MELLON UNIV	50	0	0	0	0
CHICAGO UNIV OF	85	133	203	115	177
CLAREMONT COLLEGES	- 2	0	0	0	0
CLARKSON COLLEGE OF TECH	0	66	88	75	25
COLORADO SCHOOL MINES	40	43	80	40	40
COLORADO UNIV OF	105	99	100	0	100
COLUMBIA UNIV	468	474	626	416	506
CORNELL UNIV	0	115	323	330	270
DELAWARE UNIV OF	35	46	0	0	0
DENVER UNIV OF	0	- 1	0	0	0
FLORIDA UNIV OF	49	58	50	0	0
GEORGE WASHINGTON UNIV	0	80	50	55	60
HARVARD UNIV	0	0	372	0	191
HAWAII UNIV OF	0	88	96	105	109
ILLINOIS INST TECH	53	153	80	120	100
ILLINOIS UNIV OF	385	411	414	285	737
INDIANA UNIV	0	59	85	92	90
IOWA UNIV OF IOWA CITY	55	0	0	0	0
KENT STATE UNIV	185	175	199	103	108
MARYLAND UNIV OF	35	115	132	188	196
MASSACHUSETTS INST TECH	843	795	737	926	1500
MASSACHUSETTS UNIV OF	59	65	0	70	160
MICHIGAN UNIV OF	67	0	0	60	75
MINNESOTA UNIV OF	133	129	201	303	332
NEVADA UNIV OF	0	75	87	95	98
NEW YORK CITY U - CITY CL	200	200	260	150	250
NEW YORK CITY U - QUEENS	84	81	49	0	0
NEW YORK ST UNIV OF ALBANY	88	39	136	0	62
NEW YORK ST U OF ST BROOKE	65	- 2	112	120	124
NEW YORK UNIV	1650	1400	1800	1930	2250
NORTHWESTERN UNIV	124	133	148	225	59
OREGON STATE UNIV	0	38	0	0	0
OREGON UNIV OF	0	0	103	0	0
PENNSYLVANIA STATE UNIV	91	10	0	0	0
PENNSYLVANIA UNIV- OF	0	100	169	142	25
PRINCETON UNIV	116	212	257	0	175
PURDUE UNIV	41	56	60	0	75
RENSSELAER POLYTECHNIC	91	99	150	0	98
RICE WILLIAM MARSH UNIV	45	109	249	130	218
ROCKEFELLER UNIV	79	61	53	0	80
RUTGERS UNIV	45	33	0	0	0
SOUTH DAKOTA SCH OF MINES	0	67	100	90	93
SOUTH FLORIDA UNIV OF	30	0	0	0	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
SOUTHERN CAL UNIV OF	0	0	63	70	0
SOUTHERN METHODIST UNIV	54	70	0	0	0
STANFORD LELAND JR UNVR	903	956	1077	859	1472
STEVENS INST OF TECH	0	0	0	40	0
TEXAS A & M UNIV	202	200	201	163	155
TEXAS TECH UNIV	7	0	0	0	0
TEXAS UNIV OF	263	284	336	98	720
TULSA UNIV OF	75	71	75	80	82
UTAH UNIV OF	0	100	120	132	150
VIRGINIA POLYTECHNIC INST	0	133	142	151	193
WASHINGTON UNIV OF	0	0	38	40	43
WEST VIRGINIA UNIV	0	0	0	83	0
WISCONSIN UNIV OF	289	135	177	224	350
WOODS HOLE OCNOGRPH INST	139	150	190	208	207
YALE UNIV	67	80	88	45	47

CAPITAL EQUIPMENT

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
NEW YORK UNIV	250	250	260	200	0
WISCONSIN UNIV OF	9	0	0	0	0

ADVANCED ENERGY PROJECTS

OPERATING EXPENSES

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
CALIF UNIV OF IRVINE	685	0	0	0	0
CALIFORNIA INST OF TECH	0	0	238	200	300
CASE WESTERN RESERVE U	0	0	277	300	300
CHICAGO UNIV OF	199	100	0	0	0
COLUMBIA UNIV	97	0	0	0	0
CORNELL UNIV	213	151	0	0	0
DAYTON UNIVERSITY OF	0	60	0	0	0
GEORGE WASHINGTON UNIV	0	0	294	300	0
ILLINOIS UNIV OF	120	0	413	400	200
MASSACHUSETTS INST TECH	0	417	- 14	20	0
MINNESOTA UNIV OF	0	228	0	0	0
NEW MEXICO UNIV OF	0	0	268	178	400
NORTHEASTERN UNIV	0	0	- 1	0	0
PENNSYLVANIA UNIV OF	505	101	0	0	0
STANFORD LELAND JR UNVR	0	0	- 3	0	0
STANFORD UNIVERSITY-SSRL	0	350	0	0	0
TUFTS UNIV	0	0	0	154	0
VIRGINIA POLYTECHNIC INST	105	0	0	48	0
WASHINGTON UNIV OF	0	175	216	0	300
WAYNE STATE UNIV	157	0	0	0	0

BIOLOGICAL ENERGY RESEARCH

OPERATING EXPENSES

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
BRANDEIS UNIV	41	42	49	53	57
CALIF UNIV OF BERKELEY	0	0	82	85	0
CALIF UNIV OF DAVIS	40	20	60	60	0
CALIF UNIV OF IRVINE	135	125	134	142	0
CALIF UNIV OF LOS ANGELES	134	145	168	87	87
CALIF UNIV OF RIVERSIDE	5	0	3	4	0
CALIF UNIV OF SAN DIEGO	125	125	50	0	0
CALIF UNIV OF SANTA CRUZ	46	0	0	0	0
COLORADO UNIV OF	245	270	300	351	0
CORNELL UNIV	199	213	199	163	66
FLORIDA STATE UNIV	74	116	75	0	0
FLORIDA UNIV OF	60	58	69	0	0
GEORGIA UNIV OF	434	474	603	571	414
HARVARD UNIV	55	128	120	73	0
IDAHO UNIV OF	48	58	88	73	75
ILLINOIS UNIV OF	430	495	450	471	196
INSTITUTE OF PAPER CHEM	0	44	31	0	0
IOWA STATE UNIV - AMES	0	61	54	0	0
KENTUCKY UNIV OF	0	0	28	0	71
LEHIGH UNIV	0	0	69	83	0
MARINE BIOLOGICAL LAB	0	0	20	0	0
MARQUETTE UNIV	22	16	0	0	0
MARYLAND UNIV OF	0	58	63	64	0
MASSACHUSETTS UNIV OF	75	75	77	0	0
MICHIGAN STATE UNIV	1450	1600	1730	1750	1900
MINNESOTA UNIV OF	118	158	279	178	74
MISSOURI UNIV OF	56	55	72	67	68
MT SINAI SCH OF MEDICINE	69	0	78	73	77
NEBRASKA UNIV OF	50	101	116	105	0
NEW YORK ST U OF BINGHAM	81	85	90	0	0
NORTH CAROLINA STATE U	36	0	0	0	0
NORTH CAROLINA-UNIV OF	83	80	85	87	0
NORTHWESTERN UNIV	0	0	0	60	0
OHIO STATE UNIV	64	63	63	0	0
OKLAHOMA UNIV OF	50	0	36	47	0
PENNSYLVANIA STATE UNIV	0	0	0	62	0
PENNSYLVANIA UNIV OF	79	80	80	82	83
PUERTO RICO UNIV OF	35	0	0	0	0
PURDUE UNIV	80	34	200	160	80
ROCKEFELLER UNIV	75	79	85	100	0
RUTGERS UNIV	75	120	52	55	0
SOUTHERN ILL UNIVERSITY	0	62	60	62	0
STANFORD LELAND JR UNVR	66	166	143	79	0
TENNESSEE UNIV OF	-6	0	0	0	0
UTAH STATE UNIV	75	67	81	70	0
WASHINGTON STATE UNIV	0	111	112	72	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
WASHINGTON UNIV OF	216	145	205	207	0
WASHINGTON UNIV ST LOUIS	139	129	133	65	0
WISCONSIN UNIV OF	236	277	385	320	212
CAPITAL EQUIPMENT					
COLORADO UNIV OF	150	150	100	0	0
MICHIGAN STATE UNIV	175	175	150	250	200

5. For the period FY 1981 - FY 1985, please provide, by BES subprogram and by company, actual and estimated BES funding going to industry.

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
NUCLEAR SCIENCES					
OPERATING EXPENSES					
PRINTING - DOE R&D REPORT	$- 7	$ 0	$ 0	$ 0	$ 0
ROCKWELL INTERNTL CORP	75	100	110	120	120
CAPITAL EQUIPMENT					
ROCKWELL INTERNTL CORP	0	20	15	10	0
MATERIALS SCIENCES					
OPERATING EXPENSES					
BATTELLE COLUMBUS LAB	136	142	114	160	205
BOEING AEROSPACE CO	0	0	75	0	105
FORD MOTOR CO	38	0	0	0	0
GENERAL ELECTRIC CO	166	0	0	0	0
HART FRED ASSOC	0	31	10	0	0
ROCKWELL INTERNTL CORP	196	108	195	140	350
CHEMICAL SCIENCES					
OPERATING EXPENSES					
AEROCHEM RSRCH LABS INC	85	85	71	0	0
BEND RESEARCH INC	70	74	91	90	93
CALSPAN CORPORATION	60	0	49	62	68
DYNAMICS TECHNOLOGY INC	79	80	0	0	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
FORD MOTOR CO	38	0	0	0	0
OWENS ILLINOIS INC	170	0	81	85	90
ROCKWELL INTERNTL CORP	160	155	158	0	0
SURFACE ANALYTIC RESEARCH	0	63	62	0	0
TECHNASSOCIATES INC	- 19	0	0	0	0
ENGINEERING, MATHEMATICAL AND GEOSCIENCES					
OPERATING EXPENSES					
BATTELLE COLUMBUS LAB	43	0	56	56	56
BIPHASE ENERGY SYSTEMS	65	63	0	0	0
CALSPAN CORPORATION	168	172	117	0	0
ELECTROCHEMICAL TECH CORP	0	0	69	66	83
FLOW INDUSTRIES INC	0	0	0	60	0
GENERAL ATOMIC CO	0	75	95	100	25
GEOCHEM RESEARCH	0	100	21	109	69
PHYSICAL SCIENCES INC	0	0	0	60	0
RECON	0	2	0	0	0
SCIENCE APPLICATIONS	65	65	65	157	75
SCIENTIFIC SYSTEMS	0	0	25	0	48
SKF INDUSTRIES	119	0	0	100	125
SYSTEMS ENG POWER INC	60	62	0	0	0
T.S. ASSOCIATES INC	58	0	0	0	0
WOODWARD-CLYDE CONSULTANTS	0	100	100	110	114
XDATA CORP	0	54	5	0	0
CAPITAL EQUIPMENT					
XDATA CORP	0	14	0	0	0
ADVANCED ENERGY PROJECTS					
OPERATING EXPENSES					
BATTELLE COLUMBUS LAB	0	39	0	0	0
BEND RESEARCH INC	22	430	420	135	600
DYNATECH R/D COMPANY	216	227	195	164	200
EIC LABORATORIES	0	0	134	142	100
ENERGY & ENV ENG INC	0	108	0	0	0
ENERGY & MINERALS RESH	111	0	0	0	0
FORD MOTOR CO	329	49	0	0	0
GENERAL ATOMIC CO	241	258	0	0	0
GENERAL TEL ELECTRONICS	228	243	0	0	0
GT DEVICES INC	274	285	298	300	0
MATHEMATICAL SCIENCES NW	255	255	257	250	150
MEMBRANE TECH & RES INC	0	0	84	89	400
NATIONAL TECH SYSTEMS	218	220	204	200	300
PHYSICS INTERNATIONAL	250	0	494	400	200

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
POWER CONVERSION TECHNLG	400	0	0	0	0
RADIATION MONITORING DEVICES	0	117	116	120	100
S.H.E. CORPORATION	0	121	0	0	0
SOLAMAT INC	175	295	208	200	200
SPIRE CORPORATION	46	0	0	0	0
TECHNASSOCIATES INC	- 3	0	0	0	0
WARREN WEIL ASSOCIATES	25	0	0	0	0
WESTINGHOUSE R&D CNTR	0	0	394	400	100
CAPITAL EQUIPMENT					
GENERAL ATOMIC CO	34	17	0	0	0
MATHEMATICAL SCIENCES NW	0	23	0	0	0
BIOLOGICAL ENERGY RESEARCH					
OPERATING EXPENSES					
BATTELLE COLUMBUS LAB	0	98	0	0	0
MARTIN MARIETTA CORP	80	91	86	95	0
PROGRAM DIRECTION					
OPERATING EXPENSES					
WILSON HILL ASSOC	0	30	0	0	0

6. For the period FY 1981 - FY 1985, please provide, by BES subprogram and by agency, actual and estimated funding going to support BES research at other agencies.

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
NUCLEAR SCIENCES					
OPERATING EXPENSES					
NATIONAL BUREAU STANDARD	$ 545	$ 580	$ 620	$ 630	$ 670
NAVAL RESEARCH LAB	0	0	0	120	100
CAPITAL EQUIPMENT					
NATIONAL BUREAU STANDARD	25	25	25	25	30

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
MATERIALS SCIENCES					
OPERATING EXPENSES					
NATIONAL BUREAU STANDARD	200	200	200	200	200
NATIONAL SCIENCE FOUND	0	0	0	50	0
PRINTING	0	0	2	0	0
CHEMICAL SCIENCES					
OPERATING EXPENSES					
NATIONAL BUREAU STANDARD	779	1051	1130	1199	1082
NAVAL RESEARCH LAB	65	69	0	0	0
U.S. DEPT OF COMMERCE	0	0	19	0	0
ENGINEERING, MATHEMATICAL AND GEOSCIENCES					
OPERATING EXPENSES					
NASA (JPL)	0	30	187	150	213
NATIONAL BUREAU STANDARD	0	200	350	550	600
PRINTING	0	0	0	1	0
CAPITAL EQUIPMENT					
NATIONAL BUREAU STANDARD	0	100	100	0	0
ADVANCED ENERGY PROJECTS					
OPERATING EXPENSES					
CAL TECH (JPL/NASA)	100	0	0	0	0
NAVAL RESEARCH LAB	225	0	0	0	0
BIOLOGICAL ENERGY RESEARCH					
OPERATING EXPENSES					
AGRICULTURE U.S. DEPT OF	0	0	41	43	0
NATL INST OF GEN MEDICINE	0	40	40	40	0

7. **For the period FY 1981 - FY 1985, please provide, by BES subprogram and by agency, actual and estimated funding received from other agencies to support BES research.**

Answer: No direct funding has been received from other agencies for support of BES research. A number of other agencies do support the same researchers at laboratories and universities and this does provide the BES program with a number of indirect benefits. This funding is provided direct to those institutions and researchers and the Department does not specifically track this funding.

8. **For the period FY 1981 - FY 1985, please provide, by BES subprogram and by foreign institution, actual and estimated funding going to support BES research at foreign institutions.**

Answer: Please see the table below for the requested information.

BASIC ENERGY SCIENCES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
MATERIALS SCIENCES					
OPERATING EXPENSES					
INTL ATOMIC ENERGY AGENCY	$ 38	$ 0	$ 0	$ 0	$ 0
CHEMICAL SCIENCES					
OPERATING EXPENSES					
BERGBAU-FORSCHUNG GMBH	20	0	0	0	0
INTL ATOMIC ENERGY AGENCY	0	40	0	0	0

9. **For the period FY 1981 - FY 1985, please provide, by BES subprogram and by nation, actual and estimated funding or other support received from other nations for BES research.**

Answer: The BES program has only one international agreement for which funding is formally sent to the Department via a deposit into a Treasury account. This agreement is with Japan and involves joint neutron scattering research at ORNL and BNL. The funding provided by Japan for the period FY 1981 - FY 1985 is as follows:

Year	Budget Authority
1981	$ 0
1982	0
1983	119,700
1984	180,000 (estimate)
1985	200,000 (estimate)

10. How much of the FY 1985 BES budget request is for support of programs formerly funded by the DOE Nuclear Program and any other DOE program, such as Magnetic Fusion Energy. Please enumerate these amounts by BES subprogram.

Answer: Included in the FY 1985 budget request for the Basic Energy Sciences Program is $8.4-million which is associated with program activities formerly funded in the DOE Nuclear Program.

Nuclear Sciences includes $1.4 million associated with nuclear data activities and Chemical Sciences includes $7.0 million which is made up of $2.0 million for GPE responsibility at the Argonne National Laboratory (ANL) and $5.0 million for GPP at ANL.

11. What is the BES policy towards unsolicited proposals? Is this policy uniform among all the BES subprograms, and if not, what are the differences and what are the reasons for these differences?

Answer: The BES program activity encourages unsolicited proposals and considers unsolicited proposals an essential element of the program. The policy towards unsolicited proposals is uniform among all the BES subprograms.

12. What have been the major accomplishments of the BES Program over the past five years?

Answer: The requested information is attached for 1980, 1981, 1982, and 1983. No formal report is available for 1979.

Some Examples of Accomplishments Under the Basic Energy Sciences Program during 1983

(February 15, 1984)

The Basic Energy Sciences Program supports about 1200 research projects. The following selections, while not fully reflective of the full range of activities under the program, are examples of how basic research can contribute to solving a wide variety of energy problems.

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1. Control of Structure and Properties of Ceramic Surfaces by Ion Implantation Shown

It has been demonstrated that the structure and surface hardness of ceramic surfaces can be modified and controlled by means of ion implantation to yield surface hardnesses that are greater or less than that of the original ceramic.

Results for ion-implanted alumina showed a hardness increase of 15 to 50% and a scratch-wear resistance increase of 30% as a consequence of ion implantation with chromium, nickel, iron, titanium or zirconium ions. The principal mechanism of implantation hardening was found to be due to implantation-induced structural damage on the aluminum sublattice, with some contribution from implantation damage on the oxygen sublattice.

The hardness also can be made to decrease during post-implantation thermal annealing of aluminum oxide; the mechanism was found to be associated with the recovery of the implantation-induced damage on both the aluminum and the oxygen sublattices. The implantation of alpha-phase silicon carbide with chromium or nitrogen caused the implanted surface region to become amorphous at implantation fluences above a certain critical level. This transformation from the crystalline to an amorphous state is accompanied by a decrease in hardness of 15 to 25%, an increase in fracture toughness of 30 to 40%, and an increase in scratch wear resistance of up to 70%.

This work established the feasibility of using ion implantation to systematically alter the structure and properties of ceramic surfaces. It has also demonstrated that control of the resultant structure may be achieved by the variation of implanted ion species, implantation temperature, and post implantation heat treatment.

(Oak Ridge National Laboratory, C. J. McHargue, B. R. Appleton, C. W. White, and J. M. Williams)

2. Selective Catalytic Conversion of Methanol to Ethanol Discovered

A new catalyst system has been discovered for conversion of methanol to ethanol. The system has several practical advantages over existing methods. Starting with methanol produced from coal, dry ethanol, which has higher fuel value per unit volume than methanol, is produced. The catalyst is based on iron pentacarbonyl in the presence of a tertiary amine. The principal co-product formed is carbon dioxide, rather than water as in existing methods which use a cobalt/carbonyl catalyst. Eliminating water is particularly beneficial because it can save the costly drying step.

In addition to not producing water, the iron system catalyzed reaction only requires half as much expensive hydrogen as in the cobalt/carbonyl catalyzed system. The selectivity of the iron/amine catalyst is virtually 100% for converting methanol to ethanol. There are no higher alcohols, alkyl acetates or acetals formed, in contrast to the cobalt systems, and this simplifies product purification considerably.

A mechanism for the iron/amine catalyzed reaction has been established through detailed chemical and kinetic studies. This understanding has led to development of a mixed catalyst, $Mn_2(Co)_{10}/Fe(Co)_5$/amine, which has both activity and selectivity superior to either metal carbonyl alone.

(Argonne National Laboratory, J. W. Ratkhe & coworkers)

3. Glow Discharge Implanted, Laser Annealed Silicon Single Crystals Produce Simple, High Efficiency Solar Cells

Simple, low-cost, yet very high efficiency solar cells have been produced from single crystal silicon by glow discharge implantation doping followed by pulsed laser annealing. This method involves two well understood processing steps, is easily automated and could radically change the manufacture of solar cells.

The cells are fabricated from standard phosphorous-doped single-crystal silicon wafers. A p-n junction is formed by implantation of boron followed by pulsed high-power laser illumination to activate the implanted atoms and anneal any implantation damage. A back surface field is created to reflect minority carriers back to the p-n junction area by deposition of a thin layer of antimony followed by illumination by laser pulses to cause inward diffusion. The cells are completed by cutting the wafers into desired sizes, applying contacts and antireflection coatings. The process is simple, though subtle, and efficient. It uses laser annealing and an inexpensive glow discharge boron implantation technique, both of which are easily automated and capable of high production rates. There is no high temperature processing, which is usually difficult and poorly controlled.

This development has led to three patent applications, two of which already have been granted, and the development of a XeCl laser system by an American company for automated high-production rate laser processing of these solar cells. Efficiencies of about 16.5% for these cells were measured by the Solar Energy Research Institute and found to be higher than that of any solar cell ever tested under the same conditions.

(Oak Ridge National Laboratory, R. T. Young & coworkers)

4. New Thin Film Photoelectrode Uses Visible Light to Generate Electricity or Split Water

One micron films of intrinsic (undoped) amorphous hydrogenated silicon deposited on stainless steel have been investigated as photocathodes in photoelectrochemical cells. The hydrogenated silicon was synthesized at RCA and its behavior characterized at MIT. The photoelectrodes are rugged, efficient and inexpensive.

The efficiency of the photocathode for converting visible light to electricity is in the 1-2% range, which is only about one-third less than efficiencies attained using expensive single crystal electrodes under the same conditions. Even more promising is the observation that this type of electrode produced a photovoltage more than 50% greater than that produced using a single crystal electrode. The efficiency for generating hydrogen by photoassisted electrolysis of water is equal to that obtained with the best single crystal electrodes.

Many advances reported in photoelectrochemical energy conversion in the past two years have been obtained with use of ultraviolet light, a less intense part of the solar spectrum at the earth's surface. This set of advances, in contrast, used the much more abundant visible part of sunlight. Research continues to increase further both our scientific understanding of these phenomena and the efficiencies of functioning of the new type of electrodes.

(Massachusetts Institute of Technology, M. Wrighton)

5. First Mu Meson Catalyzed Fusion Reaction Rate Measurement

In conventional approaches to fusion, hydrogen gases are heated to extremely high temperatures to form a plasma so that fusion reactions occur, releasing energy. Thirty-five years ago, it was suggested (by F.C. Frank and independently by Andrei Sakharov) that an elementary particle known as the muon could serve to catalyze the hydrogen fusion reaction so that it could proceed without the need for high temperatures. This process is therefore called cold fusion or muon-catalyzed fusion.

The basis for muon-catalyzed fusion is as follows. The negatively-charged muon behaves like a heavy electron and can substitute for an electron in a hydrogen atom. The muon is 200 times as heavy as an electron, and because there is an inverse relation between the mass of the negative particle and the radius of the atom, the muonic atom molecule is 200 times smaller than an ordinary hydrogen atom. The reduced size of the muonic atom brings the hydrogen nuclei so close together that they interact and fuse very soon after the muonic molecule forms. Indeed, the conditions inside a muonic hydrogen molecule are similar to those found inside a white dwarf star!

In this research, muons are introduced into a mixture of hydrogen gases (deuterium and tritium). Gas temperatures range from -280° F to 530° F, so the gases are very cold compared to plasmas. The muons replace electrons to form muonic hydrogen molecules and fusion ensues immediately. The muon is then free to catalyze other fusion reactions. Up to seventy (70) fusions per muon (average) have been observed in initial experiments. This is greater than expected but still insufficient for net power production. It has also been observed that the rate of the reactions increases with temperature (up to 530° F so far). However, it is clear that no thermal runaway or explosion is possible with this process.

Muon-catalyzed fusion research is continuing with Department of Energy support and similar research is also beginning in Europe and the Soviet Union. The research will provide answers to recurring questions regarding the possibility of practical applications for muon-catalyzed fusion.

(Idaho National Engineering Laboratory, S. Jones)

6. Soot Formation at Elevated Pressures Studied Using Laser Probe

Using advanced laser diagnostic techniques, considerable advances are being made in understanding the complex phenomena involved in the behavior of flames. The formation of soot, the familiar particulate matter resulting from incomplete combustion, is not only a serious source of reduced efficiency during combustion, but a potential environmental hazard as well.

Although there have been extensive studies of soot formation in combustion systems, most investigations have been carried out at normal or atmospheric pressure, despite the fact that, in practice, soot formation is most often a problem in systems that operate at high pressure. Applying advanced laser techniques, direct evidence has been obtained that soot formation increases at high pressures, not because the particles become larger, but because there are more of them.

While flames at elevated pressure are similar to those at normal atmospheric pressure, they become more compact as pressure increases. It was found that, with increasing compactness of the flame under pressure, the number of soot particles formed increases considerably. The experimental evidence comes from the much greater reduction in intensity -- by a factor of about 400 -- of a laser beam as it passes through a soot laden flame at two and one-half atmospheres of pressure compared to a soot laden flame at normal atmospheric pressure. Particle size very much affects the scattering of the laser light, and the ability to distinguish between either larger particles or more particles being responsible for the reduced beam intensity is dependent on sophisticated scattering measurements and their interpretation.

This study is typical of those now permitted by the advanced techniques for combustion research available at the Combustion Research Facility and has produced some important insight into the fundamental mechanisms responsible for the increase in soot production with pressure. Results such as these will ultimately provide the understanding necessary to control soot production in practical combustion devices operating at elevated pressure.

(Sandia National Laboratories-Livermore, W. Flower, and Stanford University, T. Bowman)

7. Highly Accurate Method for Isotope Ratio Measurements Devised Using Selective Ionization

A new, highly-selective method for measuring isotope ratios has been developed. The method, termed resonance ionization mass spectrometry (RIMS), is uniquely suited to the measurement of isotope ratios in situations where interferences from other elements are present. These interferences arise in mass spectrometry because ions are separated and detected according to mass. The problem of different atoms with the same mass occurs in both the lanthanide rare earths (e.g., cerium, used in color TV tubes, and neodymium) and actinide elements (e.g., uranium and plutonium). Resonance ionization is very selective, producing ions of only one element at a time, thus removing interferences without resorting to chemical separations or artificial measurement conditions, which seriously impair precision.

Research thus far has focused on the system cerium:neodymium:samarium (Ce:Nd:Sm) because Nd is an important element in nuclear reactor fuel burn-up analysis. Interferences from Ce (mass 142) and Sm (masses 144, 148 and 150) must be eliminated in order to arrive at an accurate isotopic analysis of Nd.

A high-powered nitrogen laser and a dye laser are used to produce light pulses of the proper wavelength to ionize Nd selectively in the presence of Sm and Ce. The ions thus formed are mass analyzed in a mass spectrometer. By switching the spectrometer back and forth between two masses, an isotopic ratio can be measured. The results obtained for isotopic ratios of Nd and Sm can be compared to the results from ordinary mass spectrometry taken under the same conditions. Errors of several hundred percent have been reduced to 1-2% with the new measurements!

(Oak Ridge National Laboratory, Dr. D. Donohue, Dr. J. Young)

8. Shear Added as a Variable to Equation of State for Fluids at Very High Flow

It has been found by techniques of molecular dynamics that in fluids, under conditions of very high flow, the equation of state includes a term involving shear as a parameter along with the usual variables of temperature, pressure and volume, necessary to define the intrinsic properties of a fluid.

Equations of state are used to predict the properties of fluids, including thermodynamic properties which are, in turn, used in the prediction of fluid behavior and the design of chemical processes. The discovery of the shear effect offers an explanation of previously unaccounted for observations of phase changes occurring under conditions of high shear. This discovery is expected to make it possible to predict thermophysical properties of complex fluids under conditions of unusual shear. Heretofore, there has been no awareness of the "shear" term because it makes essentially no contribution in the equation of state under normal conditions. Under conditions of very high flow or extreme mixing of a fluid, shear is high enough to have an effect.

The consequence of the shear effect is illustrated by the nitrogen-ethane system in which a region of non-miscibility, or a miscibility gap, is predicted by "normal" theory at given conditions of temperature and pressure, but disappears entirely when shear is taken into account. The nonexistence of a miscibility gap has significant practical consequences.

(National Bureau of Standards, H. J. M. Hanley - jointly supported by NBS)

9. The Effects of Mt. St. Helens and El Chichon Volcanoes on the Stratosphere are Significantly Different

It is known that volcanic eruptions can change climate by injecting gas and dust into the stratosphere. Of the two components, volcanic dust usually has the shorter residence time in the stratosphere (up to several weeks) while the gas, consisting mainly of SO_2, is more gradually oxidized to sulfuric acid (H_2SO_4) and other sulfates that nucleate and grow to stratospheric aerosol particles capable of affecting the solar radiation balance of the earth.

The effects of the El Chichon, Mexico eruption of 1982 and the Mt. St. Helens activity of 1980 have been sorted out from solar radiation measurements taken with a computer-controlled radiometer developed at the Pacific Northwest Laboratory.

Although Mt. St. Helens produced a large spike of SO_2, its conversion to sulfate particles was rapid and the stratospheric aerosol injection was short-lived. Consequently, no long-term effect on weather is expected from stratospheric loading by St. Helens.

The pattern of aerosol development associated with the El Chichon eruption of April 1982 was quite different. Over middle northern latitudes, where the measurements were made, the first influx of stratospheric aerosol particles did not appear until September 1982, where an abundance of sub-micron sized particles was measured. The size of the particles has since grown steadily to approach a relatively large average diameter of one micron. The larger than expected size of the sulfuric acid particles and their long residence time may well change insolation and thus have climatological consequences.

(Pacific Northwest Laboratory, J. Michalsky)

10. Wear in Sliding Friction Shown to be Due to Surface Oxidation

A wide variety of systems have components such as clutches, brakes and commutator brushes where one surface slides over another with little or no lubrication. In such systems, different types of friction induced vibrations have been frequently observed. The squeal and chatter they produce can cause excessive wear of components, severe surface damage, and fatigue failure in addition to objectionable noise levels. Research on the underlying damage mechanisms has been focussed, in particular, on interactions between friction-induced vibration and wear.

Recent experiments have shown more clearly than ever before that mild wear is due to surface oxidation. Mild wear in this context refers to wear over the range of speeds and loads normal for use of sliding contacts between metals in dry (i.e., unlubricated) conditions. The experiments showed that formation of wear particles in mild wear is localized in the oxide film formed on the surface and is due to a fatigue mechanism. Further, mild wear was shown to be a function of the system rigidity that determines the frequency of slider oscillation and, hence, the number of loading cycles. The experiments also defined the conditions leading to the transition from mild wear to severe wear.

(Illinois Institute of Technology, S. Kalpakjian)

11. Tumor Forming Gene Elimated in Widely Used DNA Vector In Plants

One of the impediments to "genetic engineering" in higher plants has been the lack of a suitable vector (a vector is an agent that can "carry" the desired gene) for transferring desirable genes into target plants. The candidate vector most studied has been a plasmid (DNA segment) deriving from the bacterium *Agrobacterium tumefaciens*. The plasmid (TI) may be used to transfer pieces of DNA carrying specific genes into host plants. Several problems exist in using this vector, however one of these is having the genetic message carried by the TI plasmid into the host expressed in the host, i.e., having the genetic message translated into a protein in the host possessing the ability to catalyze specific chemical reactions. Another is that the plasmid itself when introduced into the host plant causes tumors to develop in the plant.

Within the past year work has progressed to the point where it is now feasible by genetically altering the TI plasmid and its introduced genetic message to eliminate tumor formation (called "disarming" the plasmid). Furthermore it is also possible to demonstrate the expression of an introduced genetic character in host plant cells. Three laboratories, two in the U.S. and one in Europe, conducted these experiments, to "disarm" the TI plasmid and to demonstrate the new genetic character, independently and obtained similar results. This information brings the day closer to when it should be possible to introduce desirable traits into recipient plants with the objective of improving cultivated species.

(Washington University, M. D. Chilton)

12. Uranium Proven Unreliable Substitute for Transuranic Elements in Simulated Nuclear Waste Glass Studies

A study of simulated radioactive waste glass forms using uranium to substitute for transuranic elements has shown that they do not provide a reliable simulation of the structure and bonding properties of transuranics in silicate glasses. Since the leaching properties are dependent on bonding, this result indicates real waste systems must be investigated for reliable prediction.

To investigate the leaching behavior of radioactive waste forms, it is a common practice to study nonradioactive uranium analogs in order to simplify experimental procedures. For glass forms, air melted uranium glasses are generally studied which contain U^{6+} ions only. The assumption is made that the transuranic glasses will behave much like the uranium analogs. However, this procedure appears to be highly suspect, since transuranic glasses exhibit properties that are more similar to U^{4+} than U^{6+} glases, and the results of EXAFS and X-ray photoemission experiments, and complementary investigations of the solubility and other physical and chemical properties, have shown very different bonding characteristics of U^{4+} and U^{6+} ions in glasses. The important practical consequence of this research is that it demonstrates the unreliability of the usual simulation investigations of leaching in aqueous environments, where air melted glasses containing U^{6+} ions are used to simulate the same glasses containing transuranic elements.

(Argonne National Laboratory, D. Lam)

13. Scientific Method Established for Assessing Hydrogen Donor Capacity of Solvents for Coal Liquefaction

A new procedure has been developed to assess how effective various solvents might be as sources of hydrogen in coal liquefaction. Liquefaction of coal involves breaking chemical bonds between carbon atoms and increasing the hydrogen content to establish more liquid-like properties in the system.

Since well established chemical principles involving bond dissociation energies form the basis of the new procedure, it can be used reliably to guide the production of better hydrogen donor solvents.

In this new procedure, a reactive chemical fragment, the orthoallylbenzyl radical, is generated by thermally decomposing the chemical substance orthoallylazotoluene. In the presence of a hydrogen donor or coal liquefaction solvent, this radical can either abstract hydrogen from the donor solvent or undergo an intramolecular rearrangement reaction. The two processes form two very different hydrocarbon products. Measurement of the yield or concentration ratio of these two products allows direct comparisons to be made of the hydrogen-donor capacity of potential coal liquefaction solvents: the greater the yield of the chemical resulting from hydrogen abstraction, the better the donor capacity of the solvent.

The hydrogen donors studied thus far show expected trends of greatly increased rates of abstraction as the bond dissociation energy of the donor compound drops. The method is currently being applied to a wide variety of donor molecules and is ideal for the characterization of hydrogen donor solvent quality.

(Pacific Northwest Laboratory, J. A. Franz & Coworkers)

14. New Superconducting Shielding Method Reduces Magnetic Fields to Extremely Low Level

A new superconducting magnetic shielding method capable of reducing ambient magnetic fields to the nanogauss level has been demonstrated. This technique has the potential to revolutionize the methods of obtaining low and stable magnetic field environments necessary for low-noise operation of sensitive superconducting devices such as the Josephson Junction computer.

The method can be used to suppress magnetic fields to less than 10^{-10} Tesla, about one-half of one-millionth of the average magnetic field on the surface of the earth. This method can suppress magnetic fields more reliably and to lower values than any known technique. A very important utilization would be the shielding of such devices as computers which use superconducting elements from magnetic fields. During the necessary cooling down to operating temperatures near 4.2° Kelvin, any magnetic field may cause the sensitive superconducting circuit elements to malfunction.

This technique uses superconducting materials and some of their less obvious properties to remove and shield a region of space from magnetic fields. Superconductors exhibit the Meissner Effect: as a material is cooled below its superconducting temperature, it will expel the magnetic field. However, if the material is not a simple pure superconductor - and most practical materials are not - there will be "pinning sites" where some magnetic flux is trapped. Nearly twenty years ago, magnetic fields were shown to be quantized in units of about 2×10^{-11} Tesla. Thus each pinning site will trap an integral number of flux units. However, if a sufficient electrical current is passed through the superconductor, more than the "critical depinning current," the flux quanta become depinned and can be swept to the edge of the superconducting material.

This new superconducting magnetic shielding technique utilizes these fundamental properties to sweep the magnetic flux quanta from a long cylinder of a superconducting metal and thereby produce and maintain a region of space at the center of the cylinder at low or no magnetic field.

(Ames Laboratory, J. Clem)

15. First Measurement Made of Metallic Vapor Pressure of Einsteinium

The first measurement of the metallic vapor pressure of the man-made element number 99, einsteinium, has been made using material produced and prepared in the High Flux Isotope Reactor and Transuranium Processing Plant at the Oak Ridge National Laboratory. This is the heaviest and also highest atomic number element for which this fundamental thermodynamic measurement has been made. From the experimental data the investigators have derived a value of 31.2 kilocalories per gram-molecular weight for the energy required to vaporize the metal from a solid to a gas. This information is valuable for the increase in our understanding of the fundamental chemical and physical properties of elements and of their behavior in chemical reactions.

The measurements indicate that Einsteinium is a divalent metal, like calcium and magnesium, and thus quite unlike the lighter actinide element metals. This confirms earlier predictions based on the observed trend in the higher actinides, of the increasing stability of the divalent as compared to the trivalent state.

Einsteinium may well be the last element in the Periodic Table for which this type of measurement can be made because the next higher element, fermium, can thus far only be produced in hundred-million-fold smaller quantities.

(Los Alamos National Laboratory, J. Ward, and Oak Ridge National Laboratory R. Haire)

16. New Downhole Probe Measures Fluid and Heat Flow Simultaneously

As drilling for scientific purposes and for energy and material exploitation penetrates into rocks of increasingly hostile and variable properties, it is necessary to develop downhole measuring tools with enhanced capabilities. The measurement of heat flow in holes drilled through permeable rocks containing fluids can be a problem because it is difficult to sort out convective effects due to fluid flow from the effect of heat conduction through the rock itself. A research team focusing on new *in situ* downhole geophysical measuring techniques has developed an instrument capable of measuring and distinguishing between these two heat flow mechanisms.

The method depends on using a controlled heat source lowered into the hole to disturb the ambient heat flow regime in a reproducible way. In addition to a heat source, the instrument also has an array of temperature measuring devices (thermistors) that monitor the response of the natural environment to the artificially induced perturbation.

The response is fundamentally different for a convecting fluid system than it is for an exclusively solid rock conductor. A full three-dimensional analysis of the thermal perturbation problem allows calculation of the local fluid velocity vector and a good resolution between convective and conductive heat flow. The new probe has been successfully tested recently under field conditions at Long Valley, California, a thermally active potential target area for the Continental Scientific Drilling Program.

(Sandia National Laboratory at Albuquerque, J. Dunn)

17. Neutron "Time-of Flight" Techniques Measure Residual Stresses in Structural Materials

Neutron "time-of-flight" techniques have been used to successfully measure residual stresses in cerret materials and in a zirconium alloy. The information on cermet materials is important in the design and development of drilling inserts for oil and gas well drilling apparatus. The detailed information on residual stresses in the zirconium alloy provides valuable data for reactor fuel element and pressure tube design and performance analysis. This new non-destructive method for measuring internal residual stresses in structural alloys was developed using neutron time-of-flight measurements and its success depends critically on the high resolution powder diffractometer located at the Intense Pulsed Neutron Source at Argonne. The technique was first applied to examine the zirconium alloy tubing used as fuel cladding in water reactors. It was demonstrated that it suffers from residual tensile stresses in the circumferential direction and compression through the thickness; this combination can lead to unexpected and unacceptable creep of the cladding in service. The second application was to measure the stress level in the metallic binder phase of a hard ceramic-metal composite used as drill bit inserts for rock drilling; the high tensile residual stress found can cause premature failure of the drill bit.

This research has developed and applied a non-destructive method for characterizing quantitatively internal residual stresses. No other probe has been successful in achieving this, with the possible exception of an acoustic technique. This research will impact technically on the processing of structural materials, namely, to change these to reduce unwanted stresses and enhance desired ones. The potential economic impact is large in terms of allowing improved reactor fuel utilization in the case of the zirconium alloy and longer drill-bit life in the case of the composite noted above.

(Argonne National Laboratory, J. Faber, in collaboration with Chalk River Nuclear Laboratory, Canada)

18. Helium Atoms Found to Create Lattice Defects in Metals

A new physical process by which an impurity (helium) can produce lattice damage in metals in the absence of externally-supplied energy (i.e., thermal, radiation) has been verified experimentally. It has been known for some time that helium atoms are readily trapped in metals that have large numbers of defects in their lattice structure, e.g., as in damaged metals. More recent research has shown that helium atoms also become strongly trapped in metals with low intrinsic defect concentrations. These results stimulated calculation of lattice defects to account for the observations and have led to a model involving self-trapping of the helium. This theoretical work was followed by microscopic verification of helium-induced bubble formation in tritium charged palladium and in gold where helium was implanted at energies below the threshold that would normally cause lattice damage. In addition, evidence of helium-induced bubble formation has been found in vanadium and niobium. These latest studies have yielded new data on bubble growth processes and helium-dislocation interactions.

Thus the process of helium self-trapping in metals whereby helium forms its own lattice defects which nucleate helium gas bubbles was first indirectly inferred from experiment, then predicted by theory, and finally experimentally confirmed for four different metals and metal hydrides.

These results alter present thinking on the role radiation damage plays in helium bubble formation in metals and have shown that helium-induced degradation of metals cannot be ruled out as a potential problem area in long-term fusion energy applications. They also call attention to the possibility of future materials problems in all nuclear-based technologies. These results are directly applicable to other ongoing modelling studies of material response in fission reactor environments.

(Sandia National Laboratories-Livermore, W. D. Wilson, G. J. Thomas, and M. I. Baskes)

19. New Method to Uniformly Blend Ceramic Powders With Sintering Additives Improves Properties

A new method was developed for the homogeneous addition of sintering aids to silicon nitride powders. Sub-micron sized silicon nitride powder, when sintered, or heated under defined conditions, becomes a high-temperature structural ceramic. Sintering aids promote this process. Homogeneity of the unsintered compacts is an essential requirement in order to properly sinter silicon nitride to obtain uniform, reliable, ceramic components. The method developed is based based on the use of colloidal dispersion forces, first, to break down and prevent the formation of agglomerates in unsintered compacts of silicon nitride powder, and second, to promote mixing by causing uniform dispersion of sub-micron powder mixtures of silicon nitride and the sintering aids yttrium oxide and magnesium oxide.

A comparison of the mixing achieved by this new process with that achieved by conventional powder processing routes showed that this new method provided a dramatic improvement in the uniformity of silicon nitride unsintered compacts.

Homogeneity of the unsintered compacts containing silicon nitride and its sintering aids is necessary to produce a homogeneous flaw-free microstructure by the sintering process. Such a microstructure is required if the silicon nitride is to have good mechanical properties at 1500° C, such as for potential use in advanced turbine blades.

(Rockwell International Science Center, F. F. Lange and T. M. Shaw)

20. New Method Devised for Monitoring Thermally Enhanced Oil Recovery

The velocity and attenuation of seismic waves traveling through rocks is strongly influenced by the properties and spatial distribution of the pore fluids present. An investigation of these phenomena and their relation to bulk rock properties, pore distribution in the rock, and the presence and nature of the pore fluid, has led to a new method for reliable remote monitoring of the progress of steam flooding and other oil recovery methods. The advance results from the ability to follow changing oil temperature throughout the process. While measuring the velocity and amplitude of seismic signals as a function of pressure (up to 200 bars) and temperature (up to 150° degrees C), very large reductions in velocity (50%) and wave amplitude (7 fold) were detected when heavy-oil saturated sandstones were heated under in situ pressure conditions.

Making use of this effect, an array of seismic receivers and transmitters deployed over an oil reservoir can be used to monitor the progress of a thermal oil recovery operation. The array measures the variation of seismic velocities and amplitudes during the recovery operation, and these data can, in turn, be used to model changing oil temperature throughout the reservoir.

(Stanford University, A. Nur)

21. Improved Method Developed to Describe Crack Strain Fields in Heavy Piping and Pressure Vessels

An effective computational method was developed which permits far more realistic properties of materials to be employed in the design of major components of energy plants than allowed by current design codes. The new method which is a finite element technique, treats the deformation behavior of metals in a manner termed "incompressible-fully plastic." Though still an approximation, this is far superior to previous descriptions of strain fields around cracks in piping and pressure vessel alloys where the materials were treated as "linear elastic." With the new finite element technique, engineering calculations of the stability of a crack have been carried out under the auspices of the Electric Power Research Institute. It recently published a handbook as a reference source for solution of crack stability problems in piping and pressure vessels, which acknowledges that the calculations were made possible by the development of this finite element technique.

By providing a computational method for accurate failure analysis, this research has paved the way for proposing improved design criteria for qualifying structural components in nuclear reactors with lower initial cost than with current codes. The improved design criteria will also assist in qualifying components for continued service; the economic value of this is significant as well, given the current trend toward extending utilization of existing plants rather than building new ones.

(Brown University, R. Asaro, J. Gurland, and A. Needleman)

22. Miniaturized Thermionic Elements Introduced Into Integrated Circuits

Measurements of temperature, pressure, mass flow rates and the like often have to be carried out in an environment in which the usual instrumentation fails. Devices using semiconductors, for example, cannot be employed at temperatures above a few hundred degrees. On the other hand, devices using electron emitting elements (as in the triodes of vacuum tubes) can in principle operate well in a variety of hostile environments, but until now no way had been found to incorporate such elements in integrated circuits comparable to semiconductor microcircuits.

Recently a promising step toward solving these problems has been completed. Extremely small thermionic elements have been devised and shown to be well adapted to fabrication and use in microcircuits etched on silicon chips. Packing densities of 1000 circuit elements per square inch have been achieved and outstanding tolerance of high temperatures and radiation levels has been demonstrated. The present state of this art is not yet at its limits and further important advances are anticipated.

Unexpectedly, early results from this research have attracted the attention of a major computer products manufacturer and are being applied by that manufacturer to computer terminal display tubes. The tubes will feature an electron gun with multiple sources and built-in capability for signal processing. Although this application was not foreseen, a broad range of applications of the new integrated thermionic circuit technology is expected in the long run for instruments of interest to DOE energy and defense programs.

(Los Alamos National Laboratory, B. McCormick)

23. Unexpectedly Fast Electron Transfer Across Large Molecules Discovered

A novel set of experiments has demonstrated that electrons move surprisingly fast across large molecules. The molecules were designed with a rigid bridge separating parts of the molecule that can accept electrons at fixed, known distances. In the experiment electrons generated in a linear accelerator attach themselves at one end of each molecule and the rate at which they move to the other end is measured. Because the measured rates are extremely fast, and the spacer region is an electron insulator, it was determined electron transfer was accomplished by a "tunneling" or jumping mechanism. These results are of particular importance in the solar photochemistry research area where initial charge separation following absorption of light energy may be accomplished following such a jump.

(Argonne National Laboratory, J. Miller)

24. Neutron Reaction Cross Sections Extended By New Technique

High resolution measurements of neutron and gamma ray production cross sections have been made for the first time for neutron bombardment energies above 15 MeV. These measurements were made simultaneously over the range from 200 keV to 40 MeV using the intense pulsed beam time-of-flight system at the Oak Ridge Electron Linear Accelerator (ORELA) and were made possible by a new technique based on a high resolution lithium-doped germanium detector. Although these cross sections are of primary interest to the Office of Fusion Energy, the initial measurement provided information of timely importance to the fast reactor program, clearing up a troublesome descrepancy between experimental and theoretical results for an important design benchmark, the "large iron sphere". The measurement of the isotope iron-57 demonstrated that this minor component of natural iron (2.2% abundance) can not be ignored in the calculation. The observation of a surprisingly intense gamma-ray line, the measurement of which was made possible by the high resolution detector used, also has provided valuable information for the theorists who are developing a complicated nuclear model for the calculation of these cross sections.

The cross sections being measured with the new system are of interest not only for direct input into calculations of neutron transport and activation, but are also contributing to the development of a computational model that will permit the prediction of cross sections for high energy neutron reactions that are difficult or time-consuming to measure, but are needed for inclusion in the Evaluated Nuclear Data File (ENDF) maintained by DOE.

(Oak Ridge National Laboratory, D. Larson)

25. Elusive Energy Loss Process Affecting Fusion Verified

Measurements of dielectronic recombination, a process that has eluded experimenters for years, have finally been made. The dielectronic recombination cross sections for the doubly charged ion of boron were measured; that is the first time such measurements have been made for an ion with multiple charges.

Dielectronic recombination involves the loss of energy in a plasma and occurs when energy is absorbed by an ion when it captures an electron in the plasma. At the instant of capture, the positive charge on the ion is reduced by one unit and the resulting ion is left with excess energy. The ion next rids itself of the extra energy by the release of a photon most likely in the form of an x-ray. The net effect of all this is that the energy initially provided to effect a collision between two atoms and cause fusion of the two nuclei is instead lost through radiation. The process is important to the understanding of the behavior of plasmas and its measurement helps provide a more accurate account of the energy balance in a fusion plasma. This account in turn will permit the improved design of efficient fusion power plants.

The existence of the process was first suggested in the 1940's to account for observations made by astrophysicists to explain energy balance in stars. They could only observe the sum of several simultaneous processes, of which dielectronic recombination was one. Experimental study of the single isolated process was not possible. Now the process has been demonstrated by directing a beam of ions from an accelerator into a specially designed chamber filled with electrons. Close inspection of the interaction taking place in the chamber between the ions and electrons showed the effect sought.

While the first results are in some disagreement with theory, the fact that the process can now be studied experimentally is clearly a breakthrough in the field of high energy atomic physics and a significant contribution to our improved understanding of fusion plasma interactions.

(Oak Ridge National Laboratory, S. Datz, & co-workers)

26. Transposition of Genes in Higher Organisms Quantified for the First Time

Only recently has it been appreciated that genetic transposition (movable genes) does occur in a broad range of organisms. This phemonenon, which was discovered in maize by Dr. Barbara McClintock about thirty years ago, has never been quantified as to its rate of occurrence.

In a specially designed genetic system in maize the frequency of transposition of genes associated with the restoration of male fertility has been measured. This represents the first time that these events of movement of genes have been put on a numerical basis. Such results will assist in assessing the importance of genetic transposition and in understanding the phenomenon itself.

(University of Illinois, J. Laughnan)

27. New Method for Numerical Solution of Turbulent Combustion Model

Difficult questions in computational mathematics arising from the need to simulate real problems are being examined. One such question is a fundamental and complex problem in the area of turbulent combustion: the analysis of the effect of turbulence on the propagation of a flare. At high Reynolds number, turbulent eddies and recirculation zones form due to viscous effects. This affects the position of the flame and the distribution of unburnt fuel available for combustion. This interaction is of great importance in the design of internal combustion engines. The problem is to discover how to direct the flow in such a way that the largest amount of fuel is burned as quickly as possible, thus maximizing the force on the piston and minimizing the amount of unburnt fuel expelled at the end of a stoke.

To investigate these phenomena, a numerical technique was developed to approximate the solution of a mathematical model of turbulent combustion. This technique is specifically designed for flow at high Reynolds numbers. It portrays in a natural and effective manner the development of turbulent eddies and recirculation zones in the flow. The motion of the flame is handled in a manner that avoids the instabilities and inaccuracies that plague other front tracking techniques. The results of "numerical" experiments with this new technique on turbulent combustion in open and closed chambers show the effect of heat-producing reactions and viscosity on the rate of combustion. Heating effects along the front are seen to increase the speed at which the flame travels through the domain, decreasing the amount of time required for complete conversion of reactants to products. Viscous effects, on the other hand, both retard and accelerate flame advancement. Although the turbulent eddies produced by boundary conditions inhibit burning in corners and near walls, they also "wrinkle" the flame, increasing the surface area available for combustion. These "numerical" experiments represent a major step towards understanding the combustion process.

(Lawrence Berkeley Laboratory, J. Sethian, A. Chorin)

28. Unexpected Photochemical Mechanism Discovered in Enzyme Process for Biomass Hydrogen Production

A new photochemical route to the utilization of photons for enzymatic dissociation of water to produce hydrogen from biomass has been discovered. Experimental measurements of the simultaneous generation of hydrogen and oxygen by a laser light saturation technique have established the unexpected insight that not all photodissociation of water occurs by the same photochemical mechanism. By examining the hydrogen to oxygen ratio, it was apparent that the rate of hydrogen and oxygen generation was inconsistent with the time-accepted Z-scheme mechanism of photosynthesis. The hydrogen to oxygen ratio was found to be significantly below the 2:1 ratio of water's composition, which suggested the existence of a chemical step that encumbers the release of hydrogen. The fact that a previously unexpected mechanism exists for the enzymatic dissociation of water in biomass systems has broad implications for future developments in solar photochemistry as well as in the case of biomass photolysis.

(Oak Ridge National Laboratory, E. Greenbaum)

29. Physics Model Computations Nearly Ten Times Faster Using New Computer With Parallel Architecture

Techniques for accelerating execution of practical computational problems by using parallel processing techniques on an experimental computer have been successfully demonstrated. In mid-1983, a Denelcor HEP-1 computer was acquired as part of the DOE activity in experimental parallel architecture research.

Three problems common to the DOE activities in computational modeling were addressed: a particle-in-cell model, commonly used in plasma physics models; a hydrodynamics model, used in weapons design and combustion modeling, and a Monte Carlo model, used in modeling critical phenomena in materials and in fundarental particle physics. In each case, the problem was studied with the aim of redesigning the algorithms into sets of independent processes that could be executed concurrently. The HEP-1 architecture provides a mechanism for simultaneously executing a large number of independent processes, thereby speeding up the computation by a factor proportional to the number of processes. It was demonstrated that the computations involved in each of these modeling problems could be carried out about ten times faster with this architecture.

These results hold great promise for the design of even faster parallel architecture computers for large scale scientific computation.

(Los Alamos National Laboratory, B. Buzbee)

30. Genes Controlling the Primary Events of Photosynthesis Identified

Using molecular genetic techniques scientists have succeeded in cloning and sequencing of the nucleic acids of five genes which code for some of the first steps in photosynthesis. This work represents the first time that it has been possible to precisely locate specific genes that code for proteins involved in the primary events of photosynthesis in a structure known as a reaction center and the related "light harvesting" pigment area. This work was done with the photosynthetic bacterium known as *Rhodopseudomonas capsulata*; however, similar genes are operative in higher plants. Further, the region of common function. In this genetic material has been conserved over three billion years, the estimated evolutionary time between the bacteria and higher plants.

The significance of the work is that it permits more incisive questions to be asked about the structure and function of the biological energy conversion entity known as the photosynthetic apparatus. For example, the information on the nucleic acid sequences is easily translated in amino acid sequences in the photosynthetic proteins. That information has led to clues about how some of the components of electron transport (quinones) are attached to the proteins.

In addition, some of the proteins also have homology with those that are involved in the action of some widely used herbicides in crop production. Thus such information may also provide leads into understanding of herbicide action and possible strategy for better molecular designs of herbicides.

(Lawrence Berkeley Laboratory, J. Hearst, and K. Sauer)

31. New Techniques Developed for Analyzing Near-Surface Reactions

Two new techniques, one involving electron and photon desorption, and the other pulsed laser field evaporation have provided the means to substantially advance the understanding of atomic and molecular motion in the near surface regions of solids.

Photon stimulated desorption studies of cleaned silicon surfaces revealed that hydrogen migrating from the bulk to the surface displays a complex surface reaction resulting in the formation of hydride phases. These studies are important not only for the determination of bonding site, electronic state, and geometric configuration, but also to the technological goal of removing hydrogen from silicon.

Pulsed laser studies have shown that surface crystallography plays a major role in the catalytically important process of molecular dissociation. The temperature range over which carbon monoxide molecules dissociate has been measured, as has, for the first time, the activation energy between flat and stepped regions on the surfaces of molybdenum. These experiments showed that highly-charged field-evaporated ions are formed away from the surface after the atom has desorbed to a lower charge state.

The advances in both of the techniques will permit new insight into surface and near-surface reactions which are important to a number of technological areas.

(Sandia National Laboratory - Albuquerque, M. Knotek and G. Kellogg)

32. Dose Dependence for Defect Production Mechanism Found Using ANL High Voltage Electron Microscope (HVEM)

The unique capabilities of the Argonne National Laboratory High Voltage Electron Microscope/Tandem van de Graaff have recently been employed in attacking a controversial issue involving the nature of defects formed in the alpha-phase of iron during neutron irradiation. The basic character of the defect structure produced during neutron irradiation was reproduced by ion bonbardment and examined in situ at 40° K in the ANL-HVEM. The defect formation mechanism observed differs from what had been assumed previously, and is different from that for most other metals. It was found that the defect producing mechanism caused by high energy knock-ons (in either ion or fast neutron irradiation) changes when the dose is high enough. This research, uniquely dependent on the ANL-HVEM capability, is the first demonstration of a dose dependent change in a defect production mechanism. It will have to be included in valid models of irradiation behavior in the future and could have important consequences for predictions of radiation damage in iron and ferritic alloys. The low swelling character of these materials may, in part, be related to this newly discovered effect.

(Argonne National Laboratory, M. Kirk, and University of Illinois, I. Robertson)

Some Examples of Accomplishments Under the Basic Energy Sciences Program During 1982

(December 9, 1982)

While these selections may not reflect the full range of the basic research carried out through more than 1200 projects supported by Basic Energy Sciences, they are examples of how basic research can be brought to bear to resolve a variety of energy problems.

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1. Coexistence of Ferromagnetism and Superconductivity Observed for the First Time Using Neutron Scattering Techniques

Using neutron scattering techniques, a new phase of matter in which magnetism and superconductivity coexist has been directly observed. This work will provide a better understanding of the interaction of these two ordinarily competing forms of order in materials and may lead to better superconducting magnets and other devices through improved materials. The observation was made in a erbium-rhodium-boron compound, $ErRh_4B_4$, in the temperature range of 0.7 to 1.1° K. It has long been known to materials scientists that spontaneous ferromagnetism creates a magnetic field within the source material while superconductivity expels the magnetic field from the material. Indeed, present theories indicate that the coexistence of these two forms of long-range order in matter cannot coexist. This new investigation, carried out at Oak Ridge National Laboratory on material prepared at Argonne National Laboratory, has directly shown for the first time that ferromagnetism, along with an oscillating magnetic order, and superconductivity coexist in a narrow temperature interval at very low temperatures.

The discovery in 1977 of magnetism and superconductivity in a special class of materials containing three elements has generated considerable interest in the nature of transitions from superconductivity to magnetism, and possible coexistence of these two properties. Neutron scattering has been used at Brookhaven National Laboratory to study the magnetic transitions in a series of $(ErHo_{1-x})Rh_4B_4$ alloys (holmium replacing erbium atom for atom). $HoRh_4B_4$, the erbium compound, was found to be magnetic but not superconducting. From neutron and other measurements, Er-rich alloys were shown to be "reentrant" superconductors, that is, successively displaying paramagnetism, a property of normal metals, superconductivity and normal conducting ferromagnetism as the temperature is lowered.

$ErRh_4B_4$ shows long-range ferromagnetism at low temperatures; however, recent neutron scattering measurements on a single crystal showed the surprising result that ferromagnetism and superconductivity coexist along with an oscillating magnetic order in the small temperature range, 0.7 to 1.1° K. These studies, carried out using the unique capabilities for neutron scattering research at DOE laboratories, are proving to be of fundamental importance in understanding the interaction of magnetism and superconductivity, and have stimulated much new experimental and theoretical interest in this field.

(Argonne National Laboratory, S. K. Sinha, G. W. Crabtree and D. G. Hinks; Brookhaven National Laboratory, C. F. Majkrzak, D. E. Mounton, G. Shirane and W. Tomlinson; Oak Ridge National Laboratory, H. A. Mook; University of Maryland, J. Lynn)

2. Method for Inhibition of Intergranular Stress Corrosion Cracking Provided by Mechanistic Study

Fundamental research into causes of intergranular stress corrosion cracking (IGSCC) of structural metal alloys in aqueous solutions contaminated with sulfur species showed how borate ions inhibit the build-up of thiosulfate in a crack in the alloy and that the ratio of borate to thiosulfate ion must exceed a threshold value to inhibit cracking. This mechanistic study is providing guidance for the current evaluation of thiosulfate-ion-induced IGSCC of the nickel-base alloy used in the steam generator at the Three-Mile Island reactor TMI-1, under Nuclear Regulatory Commission support.

Iron-chromium-nickel alloys are structural engineering materials which are used throughout energy plants and are susceptible to structural changes during exposure to high temperatures. In Inconel 600, a nickel-base alloy which is the principal commercial alloy used in steam generator heat exchanger tubing in nuclear reactors, a structural change caused by improper heat treatment is the lowering of the chromium levels at the grain boundaries. When the alloy is then exposed to oxygenated water, a phenomenon known as intergranular stress corrosion cracking (IGSCC) results. In spite of the substantial efforts to understand and avoid stress corrosion of this alloy, failures continue to occur under a wide range of environmental, metallurgical and mechanical conditions.

Brookhaven National Laboratory is conducting fundamental research on IGSCC of engineering alloys in sulfur-bearing aqueous solutions. Earlier work demonstrated that the most important factor affecting IGSCC, other than oxygen level, was the ratio of the concentration of borate to thiosulfate ions in the aqueous solution. The physical basis for this appears to be that the undesirable migration of the thiosulfate into the crack is determined by this ratio through electrochemical characteristics of the ions present. At high borate/thiosulfate ratios, the protective oxide film formed on the alloy in aqueous solutions was found to be stable so the corrosion and alloy cracking tendency would be low. At low ratios, the opposite occurred due to the deleterious effect of thiosulfate on the film stability.

This fundamantal research on solution electrochemistry has provided the reactor engineering community with the basic guidelines for its assessment of sulfate-induced IGSCC in the primary heat exchangers of nuclear reactors. Understanding the electrochemistry associated with the borate ion/thiosulfate ion ratio indicated that it could be controlled by the addition of other salts to the reactor cooling water. The Nuclear Regulatory Commission is now supporting work at Brookhaven in this direction, including assessing one specific additive, a lithium-containing salt, for use in qualifying the return-to-service of the thiosulfate-contaminated steam generator at Three Mile Island TMI-1 reactor.

(Brookhaven National Laboratory, H. Isaacs, R. Newman, and K. Sieradzki)

3. Improvement in Sulfur Isotope Ratio Measurements Significant for Identifying Acid Rain Sources

Coal is plentiful but coal combustion pollutes the atmosphere. Sulfur contaminants form sulfur oxides upon burning which contribute in part to "acid rain." Sulfur emissions contain varying sulfur-32/sulfur-34 isotope ratios depending upon the source. The ratios are different for sulfur derived from microbial activity, geologic emissions, or fossil fuel combustion. Thus, the isotope ratio gives an indication of the source of the pollutant. It has been difficult, however, because of the excessively long measurement times required, to use sulfur isotope ratio determinations for source identification. In a basic research program in analytical chemistry at the Idaho National Engineering Laboratory, scientists have discovered a technique to make faster and far more precise sulfur isotope measurements.

A thousand-fold improvement has been achieved in measuring the sulfur-32/sulfur-34 isotope ratio. Previous measurements had been made by positive ion mass spectrometry. In the new technique, sulfur oxides are caused to react with fluorine to form sulfur hexafluoride. Because this is a heavier compound which easily picks up electrons, it can be readily analyzed in a negative ion mass spectrometer. With the improved sensitivity, much shorter measurement times are required and thus determination of sulfur-32/sulfur-34 isotope ratios in air is feasible.

(Idaho National Engineering Laboratory, J. E. Delmore)

4. Experimental Observation of "Hot Carriers" Could Lead to Doubling Efficiency of Photoelectrochemical Solar Devices

Photoelectrochemical systems convert solar energy to electrical or chemical energy. Scientists have developed a number of promising photoelectrochemical systems but they are far too costly for the amount of energy output. Research is being carried out at the Solar Energy Research Institute (SERI) to understand fundamental properties of photoelectrochemical systems.

A phenomenon known as "hot carrier effects" has been observed experimentally for the first time in photoelectrochemical systems. Hot carriers had been known in semiconductor solids but it was doubted that they could exist at a solid/liquid interface. Hot carriers are electrons in semiconductors which have been formed with more energy than necessary to excite the charge across the band gap. (The band gap is the difference between certain energy levels characteristic of each semiconductor.) Ordinarily, such electrons become "thermalized", that is lose energy and assume the temperature of their surroundings, before being ejected into solution. As "hot carriers" they retain some of the excess energy as they go into solution. Thus, the theoretical maximum efficiency for solar photoelectrochemical energy conversion using hot carriers is 66%, while the maximum efficiency with thermalized carriers is 31%. In addition, hot carriers can initiate chemical reactions that thermal electrons cannot.

The knowledge that hot carriers can exist at semiconductor/liquid interfaces will be useful to SERI and other scientists who are working in this area for designing more efficient photoelectrochemical systems.

(Solar Energy Research Institute, A. J. Nozik)

5. General Purpose Computer Program to Assist Human Reasoning Processes Used to Evaluate Nuclear Power Plant Systems Designs

Mathematical models of energy systems are used extensively throughout the DOE to gain insight into complex physical processes that are too dangerous, too expensive, or impossible to study experimentally. Usually, these models are solved numerically on large scale scientific computers.

Recently, researchers (computer scientists and mathematicians) at Argonne National Laboratory (ANL) have demonstrated that an Automated Reasoning Assistance Program (AURA) capable of manipulating symbolic logic equations can substantially reduce the human effort required in the analysis of complex systems, such as nuclear reactor safeguard systems and electronic circuits.

The AURA program operates on a set of general rules for manipulating logic expressions describing a complex system. Once a system is described in a suitable notation (e.g., a network of pipes and valves in a reactor cooling system), AURA is able to assist an analyst in proving that sequences of potentially dangerous events will not result in a failure of the backup system.

This theorem proving program is not specialized for one particular application. It has been used in electronic circuit design, verification of computer programs, and to solve several open questions in advanced mathematics. The ANL program is widely acknowledged to be the most flexible and powerful reasoning program yet devised.

Automated reasoning programs such as AURA have a tremendous potential in assisting humans to manage extremely complex systems of every sort, from power distribution networks to reactor systems to computer programs. Because the program provides mathematically rigorous proofs instead of numerical approximations, the results will be much more reliable and precise.

(Argonne National Laboratory, L. Wos and S. Winker)

6. Scientific Feasibility Demonstrated for Producing Batteries With Electrodes Made of Polyacetylene Sheet

The use of storage batteries in many applications has been constrained by practical limitations on size, cost and, especially, weight. An obvious example, of course, is the electric automobile. The idea that lightweight batteries might be developed from certain types of plastic materials grew out of basic scientific studies at the University of Pennsylvania on the electrochemical and physical properties of polyacetylene, an organic polymer material which can be plastically molded into any desired shape. The initial research at this basic level was supported by the Office of Naval Research, the National Science Foundation, and the Defense Advanced Research Projects Agency. The proof-of-concept research for the battery application is being supported by the Division of Advanced Energy Projects in the Department of Energy.

Chemically pure polyacetylene consists of long polymeric chains containing only carbon and hydrogen as chemical constituents. In this form, it is a good electrical insulator; however, the electrical properties of polyacetylene can be radically modified by using electrochemical techniques to introduce controlled quantities of certain other chemical species, as electrically charged ions, into the material. Depending on the concentration of these selected impurities, or "dopants", the electrical conductivity can be varied over a very wide range: from that of an insulator, through the semiconductor range and finally to values characteristic of metals. Moreover, this process is entirely reversible. In addition to being of considerable scientific interest, these remarkable properties suggested that polyacetylene could well have promise for a new type of storage battery. This was confirmed in subsequent experiments carried out by Professors MacDiarmid and Heeger at the University of Pennsylvania. The experiments indicate that plastic polyacetylene batteries have the potential of delivering ten times the power, with one tenth the weight and one third the volume, as compared with lead-acid batteries. These results led to licensing of the invention to Allied Corporation who announced plans for an intensive program of technology development.

(University of Pennsylvania, A. G. MacDiarmid and A. J. Heeger)

7. Progress Attained in Determining How Plants "Sense" Temperature

Green plant photosynthesis represents the principal mechanism by which solar energy is trapped in a form available to man. While plants are adapted to grow in many diverse niches, their growth, and concomitantly their photosynthetic capacity for solar energy conversion, is often limited by adaptation to environmental factors such as water availability, temperature extremes, salinity and numerous others. Thus if the photosynthetic base is to be expanded it is necessary to know how plants adapt to sub-optimal environmental factors.

It has been known for many years that plants may adapt, within limitations, to temperature extremes. However, one of the unanswered questions is how the plant senses temperature. We still do not know the answer to the difficult question, however, some recent insight has been achieved in investigations at Michigan State University by studying mutants of fungal slime molds which are impaired in their ability to sense temperature. The responses observed were ones where the organisms would either migrate towards or away from defined temperature regimes. The results of these studies indicate that these organisms have two sets of sensors for temperature, one at a high range, the other at the low range. The availability of these mutants also affords an opportunity to seek the molecular basis of the sensing response. Understanding the mechanism involved is important in identifying strategies for manipulating plants to expand the base of photosynthetic energy conversion by virtue of extended plant growth either by modifying ambient temperature conditions or being able to extend the use of arable land in currently less desirable temperature regions. The development of such possibilities is dependent upon the understanding of biological phenomena associated with adaptation to temperature extremes and other limiting factors. The present work is a first, but important step, in this long term effort.

(Michigan State University, K. Poff)

8. Low Temperature Neutron Irradiation Facility Provides Data Critical for Fusion Magnet Shielding Design

An important construction project in the Fusion Program, the Experimental Power Reactor (EPR), is under design and the Oak Ridge National Laboratory Low Temperature Irradiation Facility, used for neutron scattering research in materials, has been used to experimentally test the EPR magnet design. Experiments on copper, a principal component in the magnet were carried out under typical gamma ray and neutron irradiation conditions that are expected to exist in the EPR. The low temperature requirement for the experiments occurs because the magnet is a superconductor constructed with both superconducting materials and copper (normal metal) which is referred to as a stabilizer in this system. The magnet "field-on" resistivity, increases under irradiation and the designers recommended that when the increase reaches 25% of the design resistivity, the magnet should be annealed to bring it back to the initial level. They further recommended that five annealing cycles should be the lifetime maximum for the magnet. The experimental program, uniquely possible at the low temperature irradiation facility, led to the conclusion that the five annealing cycles recommended by the designers as a lifetime maximum would be reached in two years.

All recent assessments of fusion magnet materials agree that the least radiation-resistant materials are the stabilizer and the organic insulators.

The stabilizer (normal metal) of a composite superconductor safely carried the current during a localized momentary, normalization of the superconductor. The amount of normal metal needed for safe operation increases with increasing resistivity of the metal. As a result, the design of large magnets for fusion reactors will depend sensitively upon increases in the resistivity of the stabilizer produced by irradiation. To minimize these increases periodic warmup of the magnets to remove annealable portions of the radiation-produced resistivity is planned. In response to designers' needs, resistivity changes were studied in specimens of Cu throughout five cycles of an alternate irradiation (4.0° K) and annealing (14 h @ 307° K) program carried out. The results for a type of Cu now in use were used to construct the response of stabilizer resistivity to neutron dose. The gamma-ray and neutron dose scales were adjusted to match equivalent operating time at a typical magnet location in the Experimental Power Reactor (EPR). The limit of a 25% increase in field on resistivity before annealing is required was based on a consensus by designers. From the results it is concluded that the five annealing cycles recommended by designers as a lifetime maximum would be completed in only two years.

The performance data of the Cu stabilizer suggests that additional shielding for magnet protection or magnet-design changes are needed for the EPR. This information is essential for any large-scale fusion reactor design.

(Oak Ridge National Laboratory, R. R. Coltman and C. Klabunde)

9. Ion Implantation Production of Amorphous Layer on Iron Surfaces Greatly Reduces Friction

Ion implantation research has led to a non-crystalline alloy surface modification of several different iron base alloys, which have in turn exhibited superior resistance to friction and wear. Such behavior is required for the reliability of weapons systems involving coded switches, where extended life would yield a significant cost-saving benefit. It could also lead to a reduction in the necessity for the large concentrations of the strategic material chromium that is presently required for wear resistant applications, as well as an extension of the service lifetime for friction and wear resistant components.

Unlubricated friction and wear of ion implanted iron alloys is being studied in amorphous iron:titanium:carbon alloys formed by titanium and carbon implantation. This ternary amorphous layer which is formed by ion implantation was previously discovered at Sandia. Recent studies show that substantial reduction in friction (typically a factor of 2) are obtained for pure iron and for steel surfaces containing this implant-formed alloy. Also for certain alloys, the wear is strongly reduced (e.g., up to a factor of approximately 20 for light loads in 15% chromium-5% nickel steel). Interest in such surface modification treatments stems in part from important potential weapons applications involving coded switches, where extended life could be of considerable benefit. Failures during routine test operations are currently believed to be related in part to wear debris observed in post-failure inspections. Weapons requirements of reliability and minimum space prevent the use of conventional design improvements (e.g., liquid lubricants, bearings, higher torque motors). The current friction and wear studies are being carried out under analogous wear conditions to explore this important area.

(Sandia National Laboratories-Albuquerque, S. T. Picraux)

10. Detailed Measurement of Charged Particle Production by 14 MeV Neutrons Made Possible by a Specially Designed Spectrometer System

Materials bombarded by fusion neutrons are altered by nuclear transformations that produce hydrogen and helium. To assess the potential performance of specific materials for fusion reactor applications, cross-section data are required by the fusion community and the Office of Fusion Energy.

The required cross-sections are difficult to measure because of the relative weakness of available fast neutron beams, the requirement for thin targets to permit the escape of the charged particles produced, and the large radioactive backgrounds associated with fast neutrons.

In order to make much better measurements of the energy spectra and angular distributions of the charged particles under these conditions, magnetic lens systems have been developed, first at LLNL and more recently at Ohio University, to capture, focus, and transport these charged particles from the reaction target to a remote well-shielded detector.

Measurements at the high particle energy of 14 MeV encountered in fusion reactions have been completed for the materials designated to be of interest to the Fusion program, e.g., Li, Be, B, C, N, O, F, Al, Si, Ti, V, Cr, Fe, Ni, Cu, Nb, Mo, Sn, W, and Pb. The measurements made for low mass number nuclides are also of interest to others, e.g., for neutron theory studies. The detector systems have now been improved to such an extent that it has become possible to measure cross-sections at fast neutron energies other than those in the 14-15 MeV range at the very intense LLNL Rotating Target Neutron Sources where this work was carried out. Measurements have been made at the Ohio University high current tandem Van de Graaff at 8 MeV ^{58}Ni and 316-stainless steel.

(Lawrence Livermore National Laboratory, R. C. Haight; Ohio University, R. O. Lane)

11. Columbia River Basalts Found to Have Chemical Properties That Significantly Assist in Immobilization of Long Lived Radioactive Elements

The migration of elements in the earth's crust is of vital importance to understanding the possible migration of radioactive wastes from a repository to the biosphere. The chemical behavior of neptunium is being studied to accumulate information on the long term probability of radionuclide migration into the biosphere via groundwater solution and in contact with basalts. A basalt is a fine grained dark rock low in silicon and aluminum, enriched in magnesium and iron. Columbia River basalts have been found to reduce neptunium from a +6 oxidation state to a +5 or +4 state, i.e., to change its chemical behavior, so that it is highly adsorbed on the surfaces of the basalt and thus substantially immobilized and retarded with respect to entrance into the biosphere.

The iron in the basalt is in a chemically reduced state and is the active element in the basalt that reacts with neptunium. The reduction of the high oxidation state of plutonium to an immobile form by similar processes might be expected. This finding provides support for the proposed placement of deep nuclear waste repositories in basalts and suggests that ferrous-based materials might be useful as backfill to add an additional safety factor.

(Argonne National Laboratory, N. Susak, A. Friedman, S. Fried and J. Sullivan)

12. Accelerated Radiation Damage Study Shows Bulk Swelling of Proposed Nuclear Waste Storage Medium Larger Than Previously Projected

The bulk swelling of the oxide zirconolite was found to be large and in disagreement with the stability inferred from x-ray measurements. The new data may compromise the use of zirconolite in a synthetic ceramic mixture called SYNROC which has been proposed as a waste host, partly based on the earlier x-ray results. Complementary research has provided the first experimental validation of the plutonium "doping" technique, used in the zirconolite study, as an appropriate accelerated test for stability of a waste form under radiation.

A recognized need of nuclear reactor technology is the development of nuclear waste isolation methods which will be secure for geologic times (on the order of one million years) to allow decay of long-lived radioisotopes.

Ceramic waste forms potentially offer this stability. A ceramic mixture termed SYNROC (from synthetic rock) has been proposed as a waste form since it consists of crystalline materials found in nature, known to be geologically stable and capable of being tailored to be hosts for specific radionuclides. One such component, zirconolite, an oxide of zirconium, titanium, and calcium, will retain radioactive elements such as plutonium within its crystalline structure. To predict its long term behavior, it is necessary to evaluate the structural and dimensional stability of zirconolite under irradiation by the kind of radiation to which it will be subjected, in this case alpha rays.

At Los Alamos National Laboratory, zirconolite has been alloyed (or "doped") with the radioisotope plutonium-238 in order to study structural changes such as cracking or phase transitions which might compromise the stability of the waste form. Macroscopic damage has been observed in terms of bulk swelling, viz., about 5 percent swelling after an accumulated dose equivalent to that obtained in one hundred-thousand to one million years in an actual waste. In addition, x-ray measurements of lattice dilation were made for comparison with the bulk swelling. Good correlation was found initially. At higher levels of irradiation, corresponding to longer times, deviations between the bulk swelling measurements and x-ray data were found which were resolved by recognizing that the material had become amorphous and that x-rays would no longer monitor swelling correctly. This finding suggests that conclusions on the radiation stability of zirconolite based on x-ray methods alone are questionable. Specifically, the swelling of one component in SYNROC will probably lead to cracking of the entire waste form. In turn, the ingress of ground water through the cracks, which increase the surface area, will lead to leaching of the waste species by the water over that predicted. In complementary research at Pacific Northwest Laboratory, zircon (a zirconium silicate) also has been doped with plutonium and the damage measured in terms of both lattice dilation and bulk swelling. The laboratory results on doped material agreed with published data on naturally damaged zircon at low dose levels. This correlation is a critical first step in demonstrating that plutonium doping offers a valid accelerated approach to study damage accumulation in actual waste forms, with acceleration being by a factor of one-to-ten thousand over the design dose rate.

(Los Alamos National Laboratory, F. W. Clinard; Pacific Northwest Laboratory, W. J. Weber)

13. Leaching of Plutonium From Glass Host Materials Into Water Increased by High Radiation Fields

One of the mechanisms responsible over long time periods for the transport of radioactive species from one location to another is leaching. The radioactive species or any species that is soluble, is dissolved or made mobile by local groundwater and transported to some other location where it precipitates or is deposited. The extent to which this mechanism affects radioisotope movement is important in dealing with long term nuclear waste isolation. Previous studies on the effects of high radiation conditions on the rate at which plutonium can be leached out of materials have dealt with only the solid glass system and water not exposed to radiation for any extensive periods. Recent studies were conducted on an expanded system consisting of the glass which contains actinide elements and an aqueous medium in a high radiation field. These studies have shown that the strong oxidizing and reducing reactants formed during the irradiation of the aqueous medium significantly increase the amount and rate of leaching of plutonium from a standard sample of a glass material. This aspect of the effect of radiation on a glass/aqueous system was not fully recognized heretofore. It has also been shown that a significant fraction of the leached plutonium is associated with colloidal silica particles which also result from the irradiation of the glass. This association could increase the mobility of plutonium from a breached respository. The results of this research provide additional insight important in the design of nuclear waste isolation systems.

(Argonne National Laboratory, J. C. Sullivan)

14. Clarified Picture of the Chemistry of Plutonium in Environmentally Important Aqueous Media

All bodies of water contain dissolved carbon dioxide which, on solution, forms either the carbonate or bicarbonate ion. These two species are in dynamic equilibrium with bicarbonate dominating in the more acidic solutions and carbonate in the more basic ones. This dynamic equilibrium tends to maintain the acidity level in the system and is called buffering. A comprehensive picture of the chemistry of plutonium species and certain other actinides in environmentally important aqueous carbonate-bicarbonate media has been developed.

Combination of electrochemical and spectroscopic techniques has produced the first comprehensive picture of the reduction-oxidation chemistry of plutonium and certain other actinides in carbonate-bicarbonate media. Many inland lak and groundwaters are bicarbonate-buffered; and, this study has identified the environmentally important or stable oxidation states of plutonium in such media to be Pu(IV) and Pu(VI) and not Pu(V). Pu(V) has been found to be stable in the more alkaline, carbonate-buffered media found, for example, in limestone deposits. Natural reducing conditions such as iron deposits can lead to possible immobilization of the plutonium (IV), (V), or (VI) by the precipitation of Pu(III) products. Preliminary studies with uranium and neptunium show few chemical similarities with plutonium and indicate considerable complexities in actinide environmental chemistry. This new insight strongly contributes to our understanding of the behavior of actinides in the environment.

(Argonne National Laboratory, Dennis W. Wester)

15. Natural Soil Substances Shown Likely to Retard Migration of Plutonium and Other Actinides

Studies on the chemical binding of actinide elements to naturally occurring atomic materials -- organic portions of soils -- indicate that migration of plutonium through soil rich in humic materials would be very slow. Naturally occurring humic materials are polymeric sustances which are known to bind metal ions well and are found in soils and both fresh and marine waters. Data for absorption of americium, thorium, and uranium ions from aqueous solutions show that the complexing, and hence retention of these ions by the complex organic species in humic materials is strong and increases as the solution becomes more basic. Calculations of the competition for Pu(IV) - plutonium's most probable form - between hydrolysis in the aqueous solution at midrange pH values and binding to humic materials show that the binding is significantly competitive and sometimes dominant at normal environmental concentrations. Further studies of the dissociation of thorium (IV) humate show that a significant portion of the bound metal ion is essentially kinetically inert. Thus, to the extent that Th(IV) mimics the chemical behavior of Pu(IV), these results indicate a very slow migration of plutonium through soils rich in humic materials due both to the high binding constants and the very slow dissociation rate of most of the bound metal ions at low acidities. These and related studies suggest that there exists a variety of geomedia, humates as well as minerals, that adsorb and strongly bind actinides and would restrain their migration from a repository.

(Florida State University, Gregory R. Choppin)

16. Chemical Vapor Deposition Used to Produce Zirconium Diboride With Superior Solar Energy Absorption Properties

A chemically vapor deposited zirconium diboride was prepared at Sandia National Laboratories which is an oxidation resistant high temperature selective photothermal absorber. It has a desirable low infrared emittance and a high absorptivity. By virtue of its higher oxidation resistance it can function at higher temperatures that lead to a greater energy conversion efficiency, and for longer maintenance- and replacement-free lifetimes.

Recent studies on chemically vapor deposited (CVD) zirconium diboride at Sandia National Laboratories show low infrared emittance and high absorptivity, which make it attractive as a high temperature selective photothermal absorber. This research includes oxidation studies to 160° C in air, measurement of emittance and solar absorptance, characterization of antireflection coatings, and long term stability characterization in air to 600° C. Present results are that zirconium diboride undergoes slow oxidation in air above 400° C, that zirconium diboride has better spectral selectivity (emittance/absorptance ratio) than titanium diboride, that silicon nitride provides a good antireflection coating, and that the zirconium diboride/silicon nitride interface is stable in air to 600° C. Typically, a 20 micron coating of zirconium diboride is deposited by CVD on a metallic substrate and overlay an 0.07 micron antireflective film of silicon nitride on top of the zirconium diboride. As-prepared absorptance was found to be 0.87-0.93 and is 0.87 after 500 hours at 600° C. The as-prepared emittance at 100° C is 0.10 and remains the same after 300 hours at 500° C but changes to 0.16 after 500 hours at 600° C. The Solar Energy Research Institute has requested samples for further evaluation.

(Sandia National Laboratories-Albuquerque, E. Randich)

17. One-Step Route for Direct Gasification of Carbon to Methane at Relatively Low Temperature

Conversion of carbon-containing resources such as coal, woodchips, or biomass to natural gas is desirable, but the existing technology is difficult and expensive to implement. In a research program on catalysis at Lawrence Berkeley Laboratory (LBL), carbon reactions at surfaces are being studied in order to generate knowledge that might make such conversions go faster, confine them to desired products, make them easier to carry out and, thus, render them more economical. The project is jointly funded with Fossil Energy.

A promising route for direct conversion of carbon to methane has been discovered. In existing coal gasification technology, carbon is exposed to steam at high temperature to form carbon monoxide and hydrogen, which are then taken through a second step with a nickel catalyst to produce methane. Now the LBL chemists have discovered that graphite, a pure form of carbon, can be caused to react with steam at lower temperature in the presence of a potassium hydroxide catalyst to produce carbon dioxide and methane. The LBL method is attractive because it requires only one step instead of two, and it proceeds at considerably lower temperatures. These advantages point to possible savings of energy and plant equipment.

(Lawrence Berkeley Laboratory, G. A. Somorjai and N. H. Heinemann)

18. New Organometallic Chemistry May Help Coal Conversion and Industrial Chemicals

Chemical studies have led to (1) long sought-for activation of carbon-hydrogen bonds in saturated hydrocarbons, brought about by insertion of a transition metal atom between the carbon-hydrogen pair of atoms and (2) selective oxygen atom transfer to unsaturated hydrocarbons. The former may be important to activating organic groupings in coal for conversion while the latter suggests more energy efficient processes for making important chemical intermediates.

One of the greatest challenges in homogeneous transition metal catalysis involving hydrocarbons has been the activation of carbon-hydrogen bonds in completely saturated hydrocarbons. Recently, the first stable transition metal complex capable of carrying out direct intermolecular insertion of a metal center into carbon-hydrogen bonds of completely saturated hydrocarbons was discovered. An organometallic iridium hydride complex was prepared which upon irradiation with ultraviolet light underwent loss of molecular hydrogen to generate a highly reactive iridium center that inserted rapidly into the C-H bond of various hydrocarbons including saturated ones. The products have been characterized by spectroscopic techniques. Work is continuing on these reactions with attempts to develop catalytic processes for the conversion of hydrocarbons into other, more highly functionalized, organic molecules. This may be important to the activation of organic moieties in coal.

BES chemists have achieved an advance which could possibly lead to three-fold benefits in the chemical industry: large savings of energy and expense, much less wasteful use of petroleum for petrochemicals and the production of desirable chemicals which were previously difficult to obtain. These chemists have recently succeeded in preparing some palladium nitro complexes that are catalysts for the selective oxidation of various olefins to ketones or epoxides, which are important industrial chemical intermediates. The advantage of selective oxidation is that it overcomes inefficiencies in use of petroleum derived starting materials that stem from non-selective transfer of oxygen atoms from molecular oxygen to organic molecules in the catalytic cycle. A mechanism has been established for the ketone-producing catalytic cycle. It involves coordination of the olefin by palladium, transfer of an oxygen atom from the nitro complex to the olefin, separation of the product ketone and palladium nitrosyl complex and oxidation of the nitrosyl complex back to a nitro group by molecular oxygen.

(Lawrence Berkeley Laboratory, R. G. Bergman; Brookhaven National Laboratory, M. A. Andrews)

19. Experiments Impact Widely Held Theory by Showing Reaction of Oxygen Atoms With Unsaturated Hydrocarbons Does Not Involve Carbon-Carbon Bond Breakage

A turnabout has been forced on our understandings of an important aspect of combustion chemistry. Molecular beam experiments, supported by theoretical calculations, indicate that the reaction of oxygen atoms with unsaturated hydrocarbons leads preferentially to the formation of reactive species in which the oxygen atom has taken the place of another group in the molecule. Contrary to previous belief, carbon-carbon bond breaking does not occur.

Experimental investigation, under single collision conditions, of the reaction of unsaturated hydrocarbons and oxygen atom has indicated that the dominant reaction is the formation of a free radical in which an oxygen atom substitutes for another group on a carbon atom in the hydrocarbon molecule. This is contrary to previously held opinions, based on cruder experiments, that the initial step in the reaction is the breaking of a carbon-carbon bond. This research was carried out with crossed molecular beams and experiments have been performed on a number of unsaturated hydrocarbons. Theoretical calculations done in the same laboratory on the ethylene-oxygen atom reaction completely support the new experimental conclusions. These new results alter our ideas concerning the mechanism of hydrocarbon oxidation with important implications for modeling hydrocarbon combustion. The research was performed by Y. T. Lee, a recent Lawrence Award winner and his collaborators.

(Lawrence Berkeley Laboratory, Y. T. Lee and W. A. Lester)

20. Improved Understanding of Hydrogen Embrittlement Phenomenon and Methods to Prevent It Result From Ion Implantation Research

Ion implantation research at Sandia National Laboratory has led to a better understanding of the factors related to the behavior of hydrogen isotopes and helium has in several different metals. This is important for the first containing wall and limiters in magnetic fusion energy tokamak power reactors. In addition, ion implanted cesium has shown promise for inhibiting hydrogen embrittlement in stainless steels, and offers a potential solution to an old problem in other technologies.

The ion implantation program at Sandia National Laboratory is impacting on DOE magnetic fusion energy (MFE) funded program co-sited at Sandia. Two important MFE problems concerned with tokamak operation are hydrogen and helium recycle, and tritium inventory. Because a significant fraction of the tritium in tokamak power reactors will be ion-implanted from the plasma into the vacuum walls and limiters, it is important to understand the factors governing release of this hydrogen isotope from the first-wall materials. The two most important processes influencing such release are: 1) trapping of the hydrogen by implantation damage or by impurities, such as helium ejected from the burning deuterium-tritium plasma; and 2) blocking by surface permeation barriers such as oxides. Ion-beam techniques have been developed which allow trapping mechanisms and surface permeation barriers to be quantitatively characterized in a single experiment. Those methods have been successfully applied to iron, nickel and, very recently, to austenitic stainless steel, which is often used as the tokamak first-wall material. The experiments in stainless steel quantitatively measured the binding of hydrogen to helium traps and also the effectiveness of the surface barrier as measured by the recombination coefficient. These results bear directly on predictions of tritium recycling behavior in tokamaks. The mechanical embrittlement of stainless steels by hydrogen isotopes is also an important consideration in the design of nuclear weapons. This research has discovered that in nickel, which is considered to be a model system for stainless steel, ion-implanted cesium was found to strongly bind hydrogen.

If cesium can be implanted into bulk stainless steels, it could be expected to inhibit hydrogen embrittlement.

(Sandia National Laboratories-Albuquerque, S. Myers)

21. Synchrotron Radiation Used to Obtain for First Time Both Surface Structure and Temperature Distribution for Silicon on Laser Heating

Intense pulses of laser light incident on the surface of a semiconductor are known to profoundly modify its electrical and structural properties. Though this process, pulsed laser annealing, is a significant new direction for producing electronic components and photovoltaic cells, the detailed processes are not understood. The short time scale (about one one-millionth of a second) of pulsed laser annealing of semiconductors has severely limited the use of ordinary structural studies to resolve the present uncertainties concerning the detailed atomic processes. In seeking to illuminate these processes a new powerful technique has been developed to perform very fast (less than one one-millionth of a second) investigations of atomic structure utilizing the ultra-short (less than one one-billionth of a second, a nanosecond) intense x-ray pulses unique to synchrotron radiation sources. This technique, a major technological accomplishment in itself, provides three orders of magnitude improvement in the time resolution of transient structural measurements.

By synchronizing the ultra-short x-ray pulses from the Cornell High Energy Synchrotron Source (CHESS) with the 15 nanosecond pulses from the heating ruby laser, the thermally induced strain after the laser heating pulse has been observed. A thermodynamical analysis of the x-ray data has provided time-resolved lattice temperatures as a function of depth into a silicon crystal. The results indicate surface temperatures of approximately 1150 and 750° C were found 100 and 195 nanoseconds after the laser heating pulse, respectively. Large thermal gradients as a function of depth were observed, and the rapid cooling of the surface was accompanied by heat flow into the crystal, as indicated by rising temperatures deeper into the crystal.

In a second experiment, similar measurements made on silicon implanted with boron have monitored the structure of the near-surface (approximately 0.3 micron) region directly. This is possible because the surface layer is contracted due to the boron and the scattering of the x-rays is thereby displaced from that of the bulk crystal. The thermal shift of this surface scattering indicated temperatures greater than 1100° about 100 nanoseconds after the laser pulse. The disappearance of the scattering at shorter times, 40-60 nanoseconds after laser pulse show the near-surface region to be noncrystalline (melted).

Both of these experiments support the thermal model of pulsed-laser annealing over the model based on electronic processes. This result should allow more precise design of pulsed-laser annealing and accelerate its use in commercial applications.

(Oak Ridge National Laboratory, B. C. Larson, T. S. Noggle and C. W. White)

22. Molecular Clusters Generated Having Hundreds to Thousands of Molecules Bearing a Single Unit of Electric Charge

Nuclear fusion has the theoretical potential to create large amounts of energy with small amounts of raw material. The science, however, is still in its early stages of development, and although much progress is being made along promising routes, it is still worthwhile to explore other avenues. In a basic research program on mass spectrometry at the Brookhaven National Laboratory, a possible new approach to fusion has been conceived. The project is jointly funded by the Division of Chemical Sciences and the Division of Advanced Energy Projects.

Very large clusters of hydrogen molecules have been generated, each of which contains hundreds of thousands of molecules and one unit of electrical charge. These cluster ions are a new type of chemical species. Produced in a specially built mass spectrometer, they survive as long as they are not allowed to collide with other molecules. Because the clusters contain electrical charge, it should be possible to accelerate them in a properly designed ion accelerator. They can then be made to collide with solid targets or perhaps other cluster ions. This might lead to the creation of microplasmas at extremely high temperatures and thus to conditions needed for nuclear fusion.

(Brookhaven National Laboratory, L. Friedman)

23. Major Advance in Atomic Physics Permits Spectroscopic Study of X-rays Produced at Instant of Collision of an Ion and an Atom

A major advance in atomic physics has opened up an entirely new area of study: quasimolecular x-ray spectroscopy. Highly energetic atomic ions are first slowed, then collided with target atoms. At the moment of collision, x-rays are produced that can be associated with neither projectile nor target species but with a short-lived "molecule" of the two. Spectroscopy of these will add to our understanding of processes important in fusion.

A BNL physicist reports that the study of low energy multiply charged ions using the accel/decel technique has opened up an entire new field of spectroscopy of quasimolecular x-rays in collision physics. Chlorine ions, each stripped of sixteen of its seventeen electrons and having an energy of 300 keV/amu, were directed into a gas target where collisions produced x-rays that were not identifiable as belonging to either one of the atoms participating in the collision. Instead, the x-rays emitted were identified with a quasi-molecule that is formed and exists only for the period of the collision.

Previously, chlorine ions containing only one electron were produced at 4.5 MeV/amu, an energy so large that the x-rays emitted during collisions were greatly and asymmetrically broadened toward higher energy. This distortion obscured the process involving the transfer of electrons from one collision partner to the other. The x-ray structure observed at the higher energy made it impossible to assign a specific energy value to each of the x-rays produced and to detect the predicted oscillatory dependence of x-ray spectra on the impact parameter.

The new development permits a clear energy assignment to be made and allows for the oscillatory behavior to be documented. The better resolved spectra are necessary to understand the physics that takes place during the 10^{-18} sec collision which is 100 to 1000 faster than the transition lifetimes of x-rays emitted by the individual atom.

This development occurred as part of a research effort supported by Chemical Sciences in response to the needs of magnetic fusion energy technology where the physics associated with low energy highly charged ions are not well understood. The accel/decel proof-of-principle was demonstrated earlier by Jim Bayfield at the University of Pittsburgh, then under contract with the Division of Chemical Sciences. As far as is known, the BNL accelerator is the only unit in the world that can conduct this type of experiment. The only other possible competition may come from two laboratories in Germany (GSI and Heidelberg) but it is expected that they will require 3 to 4 years of development before they can obtain similar results. One of these laboratories, the one at Heidelberg, supported members of their staff to collaborate in the BNL experiments.

(Brookhaven National Laboratory, K. Jones)

24. Mathematical Theory Shows Onset of Chaotic Phenomena Follows a Precise Law Independent of Size, Boundaries, or Other System Details

Most physical systems are described mathematically by nonlinear systems of equations, including plasma dynamics, electronic circuits, and fluid flow. However, there is no satisfactory mathematical basis for describing turbulence or chaotic behavior -- usually the equations are linearized and approximations are calculated. Recently scientists at the Los Alamos National Laboratory discovered a set of universal constants that apply to a broad class of nonlinear phenomena.

In the last century, the mathematician Poincare showed that certain complex systems of differential equations are equivalent to low dimensional mappings. In studying the analytical properties of these mappings, the Los Alamos scientists were able to establish that the systems described by these equations can reach turbulent or chaotic states by evolving through a distinct, identifiable series of period doublings according to a set of universal constants. These phenomena occur regardless of the details of the specific systems. Thus in many cases what had been thought of as random behavior exhibited by these physical systems is in fact a well-determined and universal pattern. Experimental confirmation of this universal behavior has been reported in Josephson junction devices, fluid flow experiments, and chemical reactors.

Understanding the mathematical basis of turbulence and chaotic behavior is important in the study of fusion processes, combustion, fluid flow through pipes and porous media, and many other areas of interest in the development of energy systems.

(Los Alamos National Laboratory, M. Feigenbaum)

25. First Detection of Fluorescence Emission From Electronically Excited Plutonium Hexafluoride

The first detection of fluorescence emission from electronically excited PuF_6 has been achieved. This directly impacts the development of methods for the laser-based separation of plutonium isotopes.

Fluorescence has been observed in an initial study of plutonium hexafluoride vapor using visible wavelength laser excitation. This is the first observation of fluorescence from electronically excited plutonium hexafluoride. The large differences in electronic energy levels and in molecular dissociation limits make it likely that plutonium hexafluoride will not mimic uranium hexafluoride. This has been confirmed in this scouting study of selective laser excited plutonium hexafluoride.

The small fluorescence quantum yield but long fluorescence lifetime suggest that a complex mixture of energy transfer and dissociation reactions simultaneously occur when plutonium hexafluoride absorbs visible wavelength light. Experimental tests of this interpretation are being undertaken and efforts are being made to identify the emitting state. This work directly impacts on efforts to separate plutonium isotopes by providing the first information concerning the dynamics of electronically excited plutonium hexafluoride.

(Argonne National Laboratory, J. V. Beitz)

26. New Process to Recover Silver From Waste Developed Which Meets Stringent Environmental Standards

A new process for silver recovery has been developed utilizing a hypochlorite-hydrazine system that produces greater than 99.99% silver removal from spent fixer. The process not only is important for silver recovery but also meets stringent environmental standards for pollution levels of silver and cyanide in streams.

Nearly 50,000 liters of silver-bearing and cyanide-bearing waste liquids are generated annually at Oak Ridge National Laboratory from photographic and photoreproduction processes. Because the acceptable level for discharge of either silver or cyanide ions to the environment is 0.5 mg/l, a process had to be devised which was capable of both silver removal and destruction of toxic species to the desired levels. A process was developed which allows for the reduction of silver content of spent fixer from < 5g/l to < 0.5 mg/l so that the resulting effluent could be discharged directly to the streams. Silver is recovered as pure metal, no sludges are produced, and both biological oxygen demand and chemical oxygen demands are greatly reduced. The process involves the use of alkaline hypochlorite and hydrazine monohydrate through various steps that avoids the precipitation of Ag_2S which is difficult to filter. This new process is now being scaled up for production operation. A patent application has been filed and additional research on the potential use of sodium dithionite in place of hydrazine is being investigated.

(Oak Ridge National Laboratory, F. Posey and A. Palko)

27. Mathematical Description Developed of the Transition of One Stable State of a System to Two Others Has Been Applied to Combustion Processes

Understanding the complex chemical and hydrodynamical effects occurring in combustion processes is important to the design of fuel-efficient and low pollution engines. Mathematicians at Northwestern University are analyzing the mathematical properties of the large systems of equations used to model combustion processes.

Theoretical studies on flame stability have generally been based on one of two approaches: (I) the Hydrodynamical model, which accounts for thermal expansion due to combustion but ignores flame structure and (II) and diffusional-thermal model which considers flame structure in a prescribed constant density flow, thus ignoring thermal expansion. The Northwestern mathematicians derived a model in which both thermal expansion and flame structure are accounted for. They found that although plane flames are unstable to disturbances of very large wavelengths, as predicted by the Hydrodynamical model, there exists a critical wavelength below which plane flames may be stable, when diffusional-thermal effects are incorporated. The boundary between stability and instability is determined by the Lewis number, which is the ratio of thermal to mass diffusivities. When this ratio reaches a critical value, an unstable, cellularly shaped flame becomes a stable plane flame. This new, more rigorous mathematical model provides a much deeper understanding of the nature of the stability of flames.

The mathematics of combustion is vital to the understanding of experimental design and implementation, such as that carried out at the Combustion Research Facility at Sandia Livermore.

(Northwestern University, B. Matkowsky)

28. Computer Modeling Studies Support Concept of Using Heat Derived From Magma Bodies to Convert Water -- Biomass Mixtures to Gaseous Fuels

Determining the scientific feasibility of tapping hitherto unavailable energy resources from the earth is an important objective of the BES Geosciences efforts in the program area of Resources Evaluation, Recognition and Utilization.

Studies conducted at the Sandia National Laboratories (SNL-A) have demonstrated that energy derived from magma could be used to generate higher quality fuels from biomass than direct use of the biomass itself as an energy source. It has been shown that the generation of gaseous fuels using biomass as the raw material can be achieved within a magma body, at the hot rock margins of the body, or at high temperature in surface reaction vessels with magmatically derive heat from a geothermal system.

The principal gas produced in the process is methane with hydrogen as a secondary fuel. The energy content of the gaseous fuels derived from the conversion process would be about 90 to 95% the energy content of the starting biomass material, which may be a low grade material such as pulp, agricultural waste, or other cellulose containing by-products. In addition, the ability to produce high quality geothermal steam at the same time would be only slightly reduced. Thus the process would make it possible to obtain a high quality fuel while at the same time producing steam for electric power generation or other uses, enhancing the economic value of exploiting geothermal energy sources.

(Sandia National Laboratories-Albuquerque, T. Gerlach)

29. Electrical Conductivity in Oil Shale During Retorting is Orders of Magnitude Different from that of Pre- or Post-retorted Material

Studies at the Lawrence Livermore National Laboratory have shown that the electrical conductivity of oil shale during retorting is a billion times greater than its value either before or after retorting. The high conductivity results from carbon migrating to grain boundaries during retorting. Because highly conductive material inside insulators can readily be detected with radiowaves, the retorting zone of an underground body of oil shale may be mapped remotely. Such remote mapping could be more cost-effective and interfere less with the retorting process than would themocouples currently in use.

This new piece of fundamental informtion may also shed light on the question of abiogenic methane. Abiogenic methane, or methane formed from carbon and hydrogen deep within the earth's interior, unrelated to biological sources, has been proposed as a major potential source of energy. It is possible that the highly conductive layers in the earth's mantle could also be caused by carbon at grain boundaries. Such carbon, as it migrates toward the earth's surface, encounters water and could thus undergo reactions that produce methane. If such were the case, it would account for the presence of abiogenic methane in the earth as a recent product rather than as a product left over from the time when the earth was formed from primordial matter.

(Lawrence Livermore National Laboratory, A. Duba)

30. New Pathway of Energy Conversion Using Inorganic Phosphorous as a Substrate Has Been Discovered

A new pathway of energy conversion using inorganic phosphorous as a substrate has been discovered in anaerobic bacteria. This finding has been substantiated in a number of different species of bacteria. The observation is that the microbes can use the energy of pyrophosphate to support growth when carbon compounds are available as building materials. Pyrophosphate was observed to stimulate growth of otherwise slow growing organisms. The finding may result in a way of enhancing reaction rates in anaerobic digestors and sewage treatment systems to produce methane gas.

(University of Georgia, H. Peck)

31. Adaptation of Plants to Water Submersion Stress

Deep water rice represents an unusual growth adaptation mechanism and recently the way in which the plant deals with the stress of flooding has become better understood. When floating rice plants are submerged, stress-ethylene synthesis is induced. Ethylene is a growth-promoting substance in floating rice varieties. The ethylene also accumulates in the hollow stems of the plant when it is submerged. Stress-induced ethylene synthesis and accumulation of ethylene in the tissue thus appear to be adaptive mechanisms. The capacity to produce ethylene and to react to it appear only after about four weeks of growth in air. This explains why floating rice varieties have to be pregrown on dry land for several weeks before they can cope with rising flood waters. It has also been discovered that floating rices have a mechanism to conduct air along their leaf surfaces to the plant parts below the water. Once these air channels are disturbed, the underwater parts of the plant become anaerobic, and they will not survive. This explains another empirical finding, namely that a short piece of the leaf must extend above the water for the plant to survive. Examination of the leaf surfaces reveals continuous air layers trapped between hydrophobic corrugated ridges. Most gas exchange is conducted through these external air layers. Non-flooding adapted plants have air layers many times smaller. In the dark, oxygen is actually pumped down through the air layers to support respiration and in the light the air layers facilitate CO_2 absorption from the water in support of photosynthesis in submerged portions of the plant. When leaves are treated with detergent the air layers are abolished and the leaves deteriorate when submerged. Work such as this on understanding fundamental adaptive mechanisms could lead to approaches for dealing with plant growth under adverse conditions.

(Michigan State University, H. Kende)

32. Water Soluble Product From Fungal Degradation Not Previously Observed Has Been Isolated

A water soluble product from the fungal (Streptomyces) degradation of lignin has recently been isolated which is called acid precipitable polymeric lignin. The product can be recovered as more than 30% of the original total lignin. This product has not been observed previously and could serve as a potentially valuable industrial chemical for use as an adhesive or coating. A patent for this product is pending and there is interest on the part of industry.

(University of Idaho, D. Crawford)

33. Extension of Vibrational Control Theory to Operation of Catalytic Reactors

Very often the energy efficient production of various useful chemical compounds is limited by the occurrence of instabilities. These instabilities may cause the chemical process either to quench itself, thus ceasing the production; or to bring about explosive, hazardous conditions. The prevention of either extreme, while increasing the potential chemical product output is an important problem in the control of chemical reactors which is addressed at the Illinois Institute of Technology, Chicago, Illinois.

Recent advances in vibrational control theory showed how high frequency pulsations of the reactor temperature can increase the region of parameters in which stable catalytic reactor operation is obtained. This implies of course that the yield of such reactors may be significantly improved. In addition computer simulations of the operation of catalytic reactors revealed that relatively low frequency temperature oscillations also increase significantly the region of stability. This has both practical and theoretical importance. In practice varying temperatures slowly is accomplished more readily and less expensively than changing it at a high rate. From the broad theoretical point of view, low frequency vibrational control in general appears to be a relatively new and unexplored concept with potentially important consequences for control engineering.

It is expected that the new results will eventually impact positively on chemical industrial practice by permitting processes which produce chemicals at a lower energy consumption rate. Furthermore, the discovery of low frequency vibrational control should open the doors to possible new control techniques.

(Illinois Institute of Technology, S. M. Meerkov)

34. Instrumentation Developed and Demonstrated for Detection of Internal Cracks in Large Structures

Small, nearly microscopic cracks in a structure are potential precursors of a failure of the structure. Such a fracture may reach catastrophic proportions in energy-related structures, e.g., nuclear reactors, high pressure boilers, nuclear waste containers and the like. Early detection of such minute cracks presents a serious instrumentation problem which is addressed in several places, notably Ames Laboratory, Ames, Iowa.

Recent advances in the instrumentation for non-destructive evaluations permit for the first time the detection and characterization of cracks the size of a hair in many important structures. The new method features a unique combination of 1) a novel configuration of advanced high-frequency sound generators and detectors (ultrasonic transducers), 2) recent advances in theories of acoustic scattering, and 3) ingenious data processing techniques. This type of instrumentation will permit a rapid detection of cracks as small as two thousandths of an inch. It will also signal the location, dimensions and relative orientation of the cracks; information which is essential for predicting the future growth of the cracks.

The application of this new technique is expected to lead to improved assurance of fitness for service and safety of many energy-related structures.

(Ames Laboratory, J. Corones, D. O. Thompson and R. B. Thompson)

35. Have We Seen a CO_2 Warming?

A working consensus has been reached that it is not yet possible to detect the warming expected from past growth of atmospheric CO_2. Several diagnostic studies have attempted to isolate the CO_2 warming signal in the 100 year temperature record subtracting out other possible signals. Almost all studies have "seen" a CO_2 signal. However, each investigator reduced the "noise" in their own way and several derived their own temperature record. The noise reduction techniques are even in conflict. For example, one researcher requires a measure of solar variability and volcanism to isolate a signal, while another requires only volcanism and tropospheric dust to isolate a signal. Further, some key features of the data set are difficult to "fit". For example, one analysis fits the overall trend in the northern hemisphere record well, but the model does not reproduce the 1960-1975 cooling. Establishing this consensus among leaders in the field has been an important step in defining both research needs and a viable research plan.

(Lawrence Livermore National Laboratory, M. C. MacCracken)

36. Capabilities, Limitations and Prospects - Simulating CO_2-Induced Climate Change

It appears premature to draw firm, detailed conclusions from the available climate model simulations of CO_2-induced climate change. This result is based on research analyzing the capabilities, limitations and prospects of mathematical climate models. The analysis compares, primarily the General Circulation Models (GCMs) on temperature, precipitation-rate and solid moisture. These comparisons reveal similarities and differences among the GCM simulations, and some possible explanations for these differences. The models differ in their geography/orography, ocean models and solar forcing, and because, for the simulations which can be rigorously compared, either equilibrium has not been reached, or the simulated climate changes are not all statistically significant between runs within the same model. These results go beyond the recent National Academy of Sciences study in technical detail and implications for future research.

(Oregon State University, M. C. Schlesinger)

Some Examples of Accomplishments Under the Basic Energy Sciences Program During 1981

While these selections may not reflect the full range of the basic research carried out through more than 1000 projects supported by Basic Energy Sciences, they are examples of how basic research can be brought to bear to resolve a variety of energy problems.

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1. New Measurement of Californium-252 Neutron Yield Standard

The spontaneous fission of californium-252 is used as a standard against which measurements of the interaction of neutrons with nuclei, from any source, including other fissioning isotopes (e.g., uranium-235 and plutonium-239), are made. A significant nuclear data effort has produced a new and definitive measurement of the average number of neutrons emitted per fission (a parameter called nubar, $\bar{\nu}$) for californium-252. This experimental program, carried out over a period of five years, has resulted in an unprecedented accuracy for this type of measurement. The uncertainty assigned to the new value of $\bar{\nu}$ is less than 0.2%. Achieving this accuracy involved painstaking experiments and exhaustive analysis of possible experimental-errors. This new measurement, besides its fundamental importance in neutron physics research, has immediate impact on fuel cycle costs in light water reactors. The fission fuel consumption rate in reactors depends strongly on the value of $\bar{\nu}$ and more cost effective scheduling of fuel cycles and fuel enrichment can be achieved if $\bar{\nu}$ is known to very high accuracy. It has been estimated that savings of $250,000 per fuel cycle per reactor can be realized solely on the basis of the improved accuracy resulting from this work. Economies in designing fast breeder reactors should also be realized. The californium-252 used in these experiments was produced at the High Flux Isotope Reactor (HFIR) at Oak Ridge.

(Oak Ridge National Laboratory, R. Spencer, R. Gwin, and R. Ingle)

2. Theoretical Prediction of Solid State Physical Properties

As a result of recent theoretical investigations, it is now possible to calculate many structural and vibrational properties of solids using only fundamental properties of constituent atoms as input. These calculations give results within 5% of measured data for silicon and germanium and include values for the following fundamental critical parameters: lattice constants, cohesive energy, bulk modulus, shear modulus, and phonon structure. These parameters determine other macroscopic engineering properties such as strength and thermal conductivity. In addition, the studies showed, for the first time, that the temperature and pressure of solid phase transitions could also be calculated. The computations made possible by this theory are significant for conducting research on photovoltaic solar materials, catalytic properties of surfaces, and for predicting the strength and thermal stability of materials. In addition, the theory holds promise for making accurate calculations of superconducting properties important to fusion, for example, from theoretical knowledge of the interactions of electrons and phonons. This is an important step along the way to enabling the design of new materials that are tailor-made for particular applications.

(Lawrence Berkeley Laboratory, M. Cohen)

3. New Non-Destructive Downhole Seismic Source

A new downhole seismic source developed for magma exploration has enhanced our ability to define underground structures. It offers a new capability for delineating underground oil and mineral resources, and has attracted interest from oil company exploration geophysicists. The new method devised as part of a study of the energy potential of buried molten rock, employs a pneumatically-driven vibrator that operates deep within a borehole. The vibrator generates a single frequency seismic wave-train 10-seconds long. The waves travel through the surrounding formation and are received by an extensive array of surface geophones. Downhole excitation sources have always been attractive because of the direct path geometry to the geophone detectors array. The result is that ample seismic energy for convenient, reliable data collection is delivered to the formation without significant damage to the borehole. Previous downhole sources, which have been either explosives that damage the hole, or one-shot mechanical pulsers, do not enable repetitive data collection. The new approach can further be tailored to concentrate its energy into either compressional or shear waves of a desired frequency for extended duration. These different types of waves can be used to distinguish between solids and liquids. The new method has been successfully applied for its original purpose, providing measurements of seismic wave transmission through hot hydrothermal zones above partially molten rock. A new version of the seismic source, now under construction, will be compatible with standard logging cable and will have a variable frequency capability for use with more powerful sophisticated signal analysis techniques.

(Sandia-Albuquerque, H. Hardee and U. of Texas, R. Ward)

4. Basic Science Applied to Fabrication of Corrosion Resistant Intermetallic Materials

The commercial potential of a major class of materials called intermetallics was increased considerably with the development of a new fabrication technique. This was made possible from better understanding of the properties and structure of intermetallic compounds. These have ordered atomic configurations in contrast to disordered atomic configurations in metallic alloys. Because of this structural characteristic, intermetallic compounds have distinct advantages over alloys, including chemical and mechanical stability. Yet, because of their structure, intermetallics are difficult to deform without fracture.

The intermetallic Fe_3Si commercially is cast into thick wall corrosion-resistant pipe for the chemical industry where weight is not an important design consideration. Heretofore, it was not possible to produce thin wall tubing; this would require extrusion, and the Fe_3Si structure does not exhibit sufficient plasticity to avoid cracking during hot extrusion. By starting with a modified composition that could be extruded, it was found that the desired intermetallic compound could be produced through a phase change subsequent to the extrusion step; the resulting product thus has both the desired form and properties. Steel tubing clad with Fe_3Si has greater resistance to cracking under tensile loads and it was produced for the first time using conventional metal working techniques. This achievement represents a significant first step toward fabrication of thin gauge Fe_3Si intermetallic compound products for automotive and other industrial applications.

(Ames Laboratory, F. Kayser)

5. Laser Based Technique Permits Study of Critical Trace Species in Flames

Saturated absorption spectroscopy, a new laser-based technique is being used to study some of the less well understood aspects of combustion. A flame can be scanned to measure the location and concentration of highly dilute chemical species that are difficult, if not impossible, to detect by other means. This new technique holds promise for identifying and understanding the roles of dilute, but highly reactive species believed to be important in combustion. The technique uses crossed laser beams, to define a small volume element (essentially a point) within the flame. One beam is much more intense than the other. At a proper choice of wavelength the intense beam excites a large fraction of the species under study to an energy level characteristic of that species. The second beam, of the same wavelength, is much lower in intensity. If one measures absorption of the second beam when the first beam is off and then on, one finds a decrease which is proportional to the number of molecules excited by the first laser beam. Since the number of molecules excited is, in turn, proportional to the total number present, their absolute concentration can be determined after the process has been suitably calibrated.

(Sandia National Laboratory, Livermore, J. Goldsmith)

6. Predictive Model for the Ductile-Brittle-Transition-Temperature for Ferritic Steels

A major step was made toward quantitative prediction of the ductile-brittle-transition-temperature (DBTT) in ferritic steels. The DBTT is one of the least understood, yet one of the most important mechanical properties of steel. Above the DBTT, steel is tough; below, it is brittle. A semi-empirical model that incorporates both the theory of alloys and applied mechanics has been shown to have quantitative validity for binary iron alloys. It can account for the effect of different solute concentrations in these alloys on the DBTT. This is a significant first step toward understanding and controlling a property that has puzzled scientists for years. This model may lead to a capability to predict as well as explain radiation induced changes in the DBTT which now must be experimentally verified with in-reactor test coupons to assure the integrity of nuclear reactor pressure vessels.

(University of Minnesota, W. Gerbrich)

7. New Process to Recover Uranium from Leach Liquors

A new process to recover mined uranium from *in-situ* leach liquors has been developed. The new process, utilizes hydrogen peroxide. It replaces the current batch process using ammonium hydroxide, which has been virtually prohibited by EPA restrictions. These restrictions relate to the hazards to humans of ammonia ingestion from large-scale operations. The new hydrogen peroxide process is continuous and is characterized by faster filtration rates, improved separation of the uranium from contaminating metal elements such as molybdenum and vanadium, and culminates in a crystalline form of uranium peroxide particles with a narrow size distribution and low concentrations of impurities. The process is important not only for faster recovery rates, but also for its efficiency in removal of molybdenum and vanadium which adversely affect the properties of the processed uranium as a nuclear fuel. The process evolved from interaction among scientists and engineers in several different areas. When researchers knowledgeable in the surface sciences were made aware of the uranium recovery problem they devised this innovative solution to it.

(Ames Laboratory, L. Burkhart)

8. Highly Specific Extractants Synthesized for Recovery and Purification of Valuable Metals

Research started in 1980 has led to the discovery of bifunctional extractants for recovery and purification of actinides from nitric acid and from other nuclear waste solutions. They also can be used for recovery of certain valuable fission products, e.g. palladium, from high level liquid waste. This new class of bifunctional extractants, i.e. extractants which have two potential donor groups in the same molecule, are called carbamoylmethylphosphine oxides (CMPO). The carbamoyl and phosphine groups are connected by a methyl (CH_2) group. The nitrogen of the carbamoyl group has two organic groups attached to it as does the phosphorus in the phosphine group. By proper choice of these two sets of organic groupings it is possible to synthesize a CMPO which extracts americium from nitric acid solutions with a distribution coefficient greater than 20, that is, over 95% extraction efficiency. Tetra- and hexa-valent actinides are extracted with even higher distribution coefficients. Selectivity of actinides from practically all fission products is achieved by "scrubbing" with nitric acid-oxalic acid.

(Argonne National Laboratory, E. P. Horwitz)

9. New Photochemical Reaction for Producing Hydrogen

Sunlight, striking a photoelectrochemical cell containing a tungsten disulfide semiconductor electrode is a concentrated solution of sulfuric acid, will convert sulfur dioxide to sulfuric acid with the simultaneous formation of hydrogen. This photochemical reaction, which takes place with sunlight as the only energy source, occurs with 5% efficiency in normal sunlight and without degradation of the materials involved. This reaction is particularly interesting because of a known thermal reaction that decomposes sulfuric acid into sulfur dioxide and oxygen. The coupling of these two reactions would conserve sulfur dioxide and sulfuric acid; the result would be a reaction system using heat and sunlight to decompose water to hydrogen and oxygen without undesirable waste products. So far the reaction has been studied only with expensive single-crystal tungsten disulfide. Less expensive polycrystalline materials seem possible. The reaction of SO_2 to produce H_2SO_4 is also of considerable interest in the fertilizer industry.

(Massachusetts Institute of Technology, M. Wrighton)

10. Internal Friction in Car Tires - Model for Energy Loss Characteristics

A collaborative University-Industry research effort has led to the formulation of a preliminary theory of energy losses in car tires (rolling friction). In conjunction with concurrent experiments on various tire materials, this research holds promise for impressive energy savings in the transportation sector. For a long time automotive engineers have known that over 10% of the gasoline consumed in driving is lost to tires. The energy is dissipated through internal friction. Internal friction, produced as the tires flex in rolling, heats the tires, generally makes them weaker and produces no benefit. The present approach to tire design is largely a cut-and-dry process with little regard to the mechanisms for energy consumption. One reason for this has been the absence of a good model for internal friction generated in composite materials such as reinforced rubber used to construct tires, V-belts or conveyor belts. The formulation of this model provides an initial essential step towards filling this major gap in our knowledge. The starting point of this research is the theory of viscoelastic composites, i.e., modelling of the actual heterogeneous medium by a homogeneous medium such that the properties of the latter approximate reasonably well the macroscopic properties of the actual composite. Typically, tires are made of such disparate materials as rubber which flexes, stretches but is not very compressible, and cord which stretches to a limited extent under tension, but which offers little resistance to bending or compression. Both materials dissipate energy differently as the applied stress changes. Recent results have contributed to an understanding of how to combine these propetries into a single realistic model material which should be valid over a wide range of operating parameters. Thus, this theory together with the new experimental results on about 100 samples of tire materials will provide a means for predicting the internal rolling friction in a tire of a given design.

(University of Michigan, S. Clark; B. F. Goodrich Co., F. Tabaddor)

11. Microbial Synthesis of Larger Molecules from Carbon Monoxide

Methanogenic bacteria are a unique group of anaerobic organisms which have not been studied extensively. These bacteria are able to grow using carbon monoxide as a sole carbon and energy source. Racently a mutant of one bacterium in this group was found to be capable of converting carbon monoxide and other single carbon compounds to acetic acid. The significance of this discovery is that it may lead to a bioprocessing strategy for handling the unwanted gases produced in high temperature processing of biomass and coal. Such a scheme would have a two-fold advantage in disposing of waste products and at the same time producing materials which are valuable if the chemical industry. Other metabolic mutants of this organism are being isolated as an aid to understanding the pathways of metabolism involving single carbon compounds.

(University of Wisconsin, J. G. Zaikus)

12. Model to Predict the Effect of Residual Stress on Superconducting Materials

An analytical model that predicts the residual stress in superconductors has already helped fusion researchers to optimize design and fabrication of large superconducting magnets. Superconducting magnets can produce strong magnetic fields with little expenditure of energy. In general a larger supercurrent and stronger magnetic field can be obtained when the residual stress in the superconductor approaches zero. The model predicting residual stress requires only knowledge of the volume fraction of each component in the composite conductor where, for example, the superconductor is Nb_3Sn and the other components are Nb, Cu and Ta. Thus different proportions of components give different residual stresses, and the selection of materials for producing an optimum superconductor must consider minimizing the residual stress obtained for that choice of materials. This selection process can now be done analytically rather than by the past "cut and try" experimental approach.

(Oak Ridge National Laboratory, D. Kroger, C. Koch, D. Easton)

13. Irradiation Stability of Ceramics for Radioactive Waste Disposal

Materials used for storage of high level radioactive waste must be mechanically stable over geologic periods to insure that no hazardous material escapes into the biosphere. A relatively new concept for storage is the use of synthetic rock to sequester the most hazardous species. Synthetic rock is a man-made ceramic material modeled after minerals that are known to be stable for a very long time. An experimental program in cooperation with Australian scientists has been examining the resistance to radiation effects of a candidate mineral, hollandite, which is theoretically attractive for storing cesium, one of the most hazardous species. Hollandite was exposed to the equivalent of 1,000,000 years of radioactive decay in laboratory experiments using an accelerator. The experiments showed that hollandite did not crack or experience a significant volume change, thereby suggesting validity of the "synrock" concept. Other mineral structures known to exhibit long term geologic stability, and having atomic structures compatible with the longest lived components in radioactive waste, will be studied with the goal of developing a design methodology for synrock waste host materials from several compatible mineral phases.

(Battelle Pacific Northwest Laboratory, W. J. Weber)

14. Fracture in Ductile Metal Observed by Microscopy

Fracture in ductile metal is of great practical importance. This phenomenon was investigated under high resolution electron microscopy, and for the first time, fracture was photographed as it actually took place. Photographs of aluminum under tensile stress in the electron microscope were taken. The aluminum sample appeared to fracture as a result of two mechanisms, one involving stress, and the other failure in a dislocation-free zone. The latter observation is new. It offers insight into the understanding of the fracture of ductile metals, and will assist in the design of ductile alloys with higher resistance to fracture.

(Oak Ridge National Laboratory, S. M. Ohr)

15. Dynamics of Molecular Ions Now Accessible Through Controlled Coulombic Fragmentation

A new technique now permits the experimental determination of the structure and binding forces in molecular ions. These ions are extremely reactive species that can have profound effects on chemical reactions. This great reactivity has made it impossible to determine the structural and binding characteristics of molecular ions except in a few rare situations. The ion studied is accelerated and passed through a thin crystal, which gently strips electrons from the ions. This leaves constituent atoms positively charged, so that electrostatic repulsion breaks the ion apart. As the constituent charged atoms separate, the time and place of detection of these fragments are determined and can be used to calculate a series of "snapshots" of the ion as it disintegrates. This information in turn reveals the forces binding the atoms together in the ion. Among processes that can benefit from this knowledge are the direct conversion process in MHD and studies of energy loss mechanisms in fusion plasmas.

(Argonne National Laboratory, D. S. Gemmell, R. P. Kanter)

16. Fluorescence of Actinides: Highly Sensitive Monitoring Technique

Clever choices of laser excitation frequencies have enabled measurement of fluorescence spectra and lifetimes of actinides in aqueous solution. This may make possible routine monitoring of actinides in process chemistry and in the aquatic or geologic environment. Early studies of actinide emission spectra had indicated that the fluorescence spectrum and lifetime of curium species in the -3 valence state should be observable but not those of other +3 actinides. The curium (+3) fluorescence has now been measured in remarkably dilute concentrations of about 10^{-9} molar. Further detailed studies using carefully chosen laser excitation have now shown that similar observations are also possible for einsteinium (-3), and almost certainly for berkelium (-3) and americium (-3). These techniques are being extended to other valence states of the actinides so that similar information can be obtained for uranium, neptunium, and plutonium. Since the energy and lifetime of fluorescence radiation is highly sensitive to the identity of the actinide species and its valence state, this information may lead to the development of powerful techniques for monitoring actinides.

(Argonne National Laboratory, J. Beitz)

17. Change in Catalyst Substrate Dramatically Changes Fuel Product

Preliminary experimental results have dramatically shown that the specificity of the catalytic conversion of coal synthesis gas ($CO + H_2$) to methanol and methane is dependent on the type of silica substrate used to support the palladium metal catalyst. Palladium on Grade-57 gel was almost 100% selective in catalyzing the formation of methanol whereas palladium on Grade-01 gel had 100% selectivity to methane. Palladium on Cab-O-Sil was found to produce both fuels. The significance of this discovery is knowledge that the ability of the palladium to catalyze the synthesis of methanol is not an inherent, general property of the metal alone. This is one of the most dramatic examples known of a substrate effect in heterogeneous catalysis. Research is in progress to explain this observation, which may strongly influence the use of synthesis gas from coal.

(Texas A & M, J. H. Lunsford)

18. Coal and Oil Shale Non-Destructively Analyzed for Organic Matter

Valuable samples of coal solutions and oil shales were subjected to rapid non-destructive tests based on small angle scattering of neutrons. One objective was to learn if this technique could be used to physically characterize the samples prior to other necessary, but destructive tests. Very useful results were obtained: the concentration of coal in solution could be measured over a dynamic range of 10 and the size and shape distribution of pores in oil shale determined. Contrary to earlier assumptions, it was learned that the pores did not flatten with increasing lithostatic pressure (depth). Indeed, there does not seem to be a clear correlation between pore size and depth which means that specific site-depth testing is required before deciding how to extract oil from oil shale on a large scale basis. The neutron technique is extremely efficient requiring only a few hours for a full analysis and can cover a wide range of solution concentrations and pore configurations.

(Oak Ridge National Laboratory, G. D. Wignall, H. R. Child)

19. Long Term Stability of Nuclear Fuels

Long-term stability of reactor fuel elements is important for safety and economics in the nuclear industry. One of the most important stability factors for UO_2, the most widely used fuel, is slow buildup of oxygen gas during power generation. Oxygen pressure and how quickly oxygen can migrate to the cladding (diffusion) determine fuel element stability. An ingenious technique to measure the diffusion coefficient of oxygen in UO_2 was devised. It is based on measurement of oxygen isotope ratios in isotopically enriched wafers of UO_2 that are separated by a thin membrane of molten uranium. Results from this experiment indicate that the diffusivity of oxygen in UO_2 is 100 to 1000 times less than had been estimated from previous experiments. This experiment establishes more reliable values for the thermal properties governing the stability of UO_2 fuel elements.

(Lawrence Berkeley Laboratory, D. Olander)

20. Studies of Sulfate Pollutant Related to Acid Rain Sources

In an extensive set of experiments to characterize aerosols, it was found that sulfates produced in burning fossil fuel were richer in oxygen-18 than were sulfates produced in the atmosphere. Oxygen isotope radio measurements were subsequently made to determine primary and secondary sulfates in airborne sulfate samples and in snow and rain, and have resulted in new estimates of their concentrations. Primary sulfates are defined as sulfates that are formed before emission into the atmosphere as from fossil plants; secondary sulfates are formed after emission of sulfur into the atmosphere. Primary sulfates collected in the Chicago area from snow and rain were found to have a higher concentration by 4-5 over that previously accepted. These new findings indicate that previous assumptions concerning acid rain sources need to be reexamined. Further, the new isotopic analysis method should prove invaluable in U.S. and international programs to characterize acid rain and its sources.

(Argonne National Laboratory, B. Holt, R. Kumar, P. Cunningham)

21. Electromagnetic Measurements Track In Situ Oil Shale Retorting

Measurement of the electrical conductivity of oil shale in small scale aboratory experiments has led to a new phenomenological model that predicts conductivity changes during underground retorting of oil shale. The model was developed with the idea of obtaining remote underground images from high frequency electromagnetic measurements.

With the help of this new development, field experiments in an underground oil shale retort were designed and conducted. In this field experiment, sponsored by Fossil Energy, the new electromagnetic measurements were compared with measurements obtained with a more expensive and cumbersome method involving an array of thermocouples placed in the retort. The results indicate the electromagnetic method is not only cheaper but also more reliable. It is now possible to remotely pinpoint the location of an underground oil shale retort and simultaneously determine the temperatures in the retort zone.

(Lawrence Livermore National Laboratory, A. Duba, W. Daily, R. Lytle
A. Piwinskii)

22. Vibrational Control for Increasing Productivity of Chemical Reactors

Controlled oscillation of the flow of chemicals into many chemical reactors can give as much as a five-fold increase in production rate over the rate practical without the oscillations. This new insight came from applying the concepts of vibrational control to continuous stirred tank chemical reactors, widely used to carry out heat producing reactions such as ammonia synthesis. Vibrational control is fundamentally different from feedback control; a simple physical example is stabilization of a rigid pendulum in a normally unstable upright position by oscillation of its point of suspension. Lasers and particle accelerators are currently often operated with vibrational control. The processes run in continuous stirred tank chemical reactors frequently suffer from product decomposition (or recombination) at normal operating temperatures. These problems can be minimized, according to the new theoretical developments, by oscillations which allow stable operation at lower than usual temperatures and higher than usual flow rates. Experiments are underway to demonstrate the method and explore its range of potential applications.

(Illinois Institute of Technology, S. Meerkov)

23. Production of Oxygen Enriched Air Using Liquid Membranes

A significant new development uses a liquid membrane to provide oxygen enriched air (80% O_2) in a single step. It is several times superior to any other membrane process. In this new approach, a liquid carrier binds oxygen on one side of the membrane and releases it on the other, in a way that is similar to hemoglobin. There are indications that this purification system has excellent stability and that recycling of the enriched product will result in nearly pure oxygen. Combustion accounts for over 90% of the U.S. energy consumption. The presence of nitrogen in combustion air (80% N_2) gives rise to a substantial energy loss in heating nitrogen and to air pollution by oxidation of nitrogen at high temperature. Both adverse effects can be reduced by enriching the air needed for combustion with oxygen. Many industrial processes also require nearly pure oxygen which is obtained by fractional distillation of air. The new process could lead to a more economic alternative. This research, is being transferred to the Division of Coal Gasification, Office of Coal Processing for further development.

(Bend Research, Inc., H. Lonsdale)

24. Use of Microorganisms to Remove Sulfur and Nitrogen from Fossil Fuels

The number of petroleum sources containing levels of nitrogen and sulfur contaminants low enough so that combustion of this fuel does not lead to significant environmental pollution is rapidly decreasing. Stocks of more heavily contaminated petroleum are in good supply and could satisfy a considerable portion of our energy needs if inexpensive and efficient methods for the removal of these contaminants were available. One approach to this problem is through biological purification of petroleum. More than ten isolates of bacteria which attack a number of organic nitrogen- or sulfur-containing compounds found in petroleum or synfuels have been obtained from soils and other sources. The bacteria were found to be capable of converting up to 98% of some of the contaminants to water-soluble products within 2-3 days. In the water-soluble form the contaminants can be removed readily. The bacteria carry out the oxidation of these compounds with a high degree of selectivity leaving the useful hydrocarbons unaltered. The bacterial genetic elements controlling these capabilities have been found to reside on plasmids, suggesting very favorable potential for applying genetic engineering techniques leading to a new biotechnology for decontaminating petroleum.

(University of Georgia, W. R. Finnerty)

25. Hydrogen Fluoride Used to Convert Celluose to Sugar

A simple economic method of "cracking" cellulose to yield feedstock sugars remains elusive. In exploring a novel cellulose "cracking" method that uses gaseous or liquid anhydrous hydrogen fluoride, several clear advantages over conventional acid hydrolysis techniques were discovered. The hydrogen fluoride technique gave higher sugar yield than other acid hydrolysis procedures. It is a process that is faster, more simple and consumes less energy. Furthermore, it appears that most of the hydrogen fluoride can be recycled. These encouraging experiments carried out on a bench top scale need further optimization before scale-up can be contemplated.

(Michigan State University, D. Lamport)

26. Key Developments In Plant Molecular Biology

Two recent advances involving studies on the structure and function of plant genes requisite to the development of the "genetic engineering" of plants have been made. The studies are being done on maize which is one of the most important model systems for plant molecular biology. The rapid sequence determination of the nucleotide base "building blocks" in maize genes has been accomplished by the application of methods modified from those used in microbial systems. The second advance concerns the biochemical localization of a "control element" gene as a prelude to cloning it. Control elements are of great significance because they act to turn on and turn off, in a highly precise way, other genes which govern a variety of biochemical functions. Control elements are believed to act by the insertion of specific DNA sequences into particular regions of the chromosome. These advances should lead to the further development of methods to convey specific desired genes from one plant to another as well as the capability of bringing about specific alterations in plant genes as might be desired in the development of biomass producing plants.

(Brookhaven National Laboratory, B. Burr, F. Burr; University of Minnesota, J. Messing)

27. Coated Semiconductor Electrode Improves Possibility of Electrochemical Solar Cell

A new technique has been developed for electrodepositing a polymer film of polypyrrole on a polycrystalline n-type silicon semiconductor electrode. The treated electrode was used as the anode (positive electrode) in a cell containing a water solution of iron salts and an ordinary metal cathode (negative electrode). Upon illumination with visible light the iron was oxidized at the anode and reduced at the cathode, so that with no net change in the solution, electricity flowed in an external circuit. Untreated electrodes corrode sufficiently in a few seconds of operation to stop the flow of electricity. Initial tests of these coated electrodes were run for 120 hours with little change in their performance. Tests of power conversion indicated a 3% conversion efficiency, about one third that of a solid state device employing polycrystalline silicon. The important characteristics of this coating are its complete coverage of the electrode (providing the protection) and its high electrical conductivity (providing a path for the flow of electricity). Current research is exploring the properties of the polypyrrole film, its use to protect other semiconductor electrodes and its use in fuel-forming photoelectrochemical cells.

(Solar Energy Research Institute, A. J. Nozik, A. J. Frank, R. Noufi)

28. Breakthrough Experiment Measures Electron-Electron Interactions

Laser beam probing of energetic negative hydrogen ions (H^-) has led to the first precise measurements of the interaction between two electrons in the isolated ion. The experiments used the LAMPF ion beam to provide H^-, a species not commonly accessible by conventional laboratory methods, and a laser. The angle between the ion beam and the laser beam could be accurately controlled, so that the frequency (energy) of the photons in the moving reference frame of the ions could be varied. This phenomenon, called the Doppler effect, is commonly experienced when a stationary listener hears the frequency of a siren change as the siren approaches and then recedes from the listener. In the experiment, the energy range in which strong photon absorption (resulting in electron emission) took place was larger than that predicted by theory. This suggests that some physics was omitted from the mathematical formulation describing the H^- system. The new experimental results will aid in understanding the role of electron correlation (how electrons affect each other) in H^- and should stimulate new ideas toward better understanding of more complex ions. Examples are the highly ionized heavy atoms that contaminate fusion plasmas. Also, the negative hydrogen ion is of great practical interest because it is a desirable precursor to formation of neutral hydrogen beams that provide auxiliary heating of fusion plasmas.

(University of New Mexico, H. Bryant)

29. Two Discoveries Strengthen Scientific Basis for Catalyst Design

A better understanding of the detailed bonding interaction between the transition metals which are used as catalysts and substrates for synthesis gas ($CO + H_2$) conversions has resulted from two recent scientific discoveries. In the first, convincing evidence has been obtained favoring one of three proposed mechanisms for hydrocarbon chain growth in Fischer-Tropsch synthesis. The results clearly indicate that the chain growth occurs by insertion of CH_2 species into a metal alkyl bond. This insight is an important contribution to the design of catalysts of high specificity for conversion of synthesis gas into longer chain hydrocarbons. In the second, recent work has resulted in a kinetic method for obtaining values of metal-carbon bond strengths. These are very important in catalytic reactions involving the formation or isomerization of hydrocarbons. It has recently been shown that a kinetic method can be used to obtain values for chromium-carbon bond energies. Values for the energies of bonds between chromium and hydroxyalkyl groups have been obtained by measuring both forward and reverse rates of α-hydroxyalkyl metal-carbon bond reactions. These particular bond energies are especially important since hydroxyalkyls are believed to be intermediates in catalyzed $H_2 + CO$ reactions which lead to hydrocarbon and oxygenated hydrocarbon products (Fischer-Tropsch synthesis).

(University of Texas, R. Pettit; Ames Laboratory, J. H. Espenson)

30. Mathematical Models of Turbulence

Turbulence in fluid flow is a complex and poorly understood phenomenon; but it is crucial in determining efficiency in combustion processes. This year a major breakthrough was made in solving the nonlinear differential equations that describe turbulence. New numerical methods were applied for the first time to provide accurate solutions to classes of energy related problems that were previously intractable using standard methods. Researchers supported by Applied Mathematical Sciences successfully modeled the combustion of gases in a cylinder and compared the numerical results with photographs obtained in laboratory experiments. The turbulent behavior of the combusting mixture is duplicated by the mathematical model, providing direct evidence that the model is accurate and that the numerical techniques are stable. These techniques can now be applied to more realistic geometrical configurations, such as engines, to provide more efficient and pollution-free designs.

Recently, mathematically similar techniques were applied to the "fingering" phenomenon that occurs when water or steam is injected into an oil reservoir for tertiary recovery. Fluid instabilities develop that cause the injected fluid to break through the oil too soon, limiting the amount of oil that can be recovered.

Unforeseen but valuable spinoffs in apparently unrelated areas are common to mathematical research. This was amply demonstrated by the application of the turbulence modeling methods to explain how valves in the human heart are closed as a result of vortices in the turbulent flow of blood, when it appears that the valves are too weak to close with their own muscle power.

(Lawrence Berkeley Laboratory, A. Chorin; Courant Institute of NYU, J. Glimm)

Some Examples of Accomplishments Under the Basic Energy Sciences Program During 1980

These selections do not necessarily reflect the full range of the basic research carried out through more than 1000 projects supported by Basic Energy Sciences.

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1. Fission Product Iodine Release in Nuclear Accidents

The release of fission product iodine as the result of a reactor core meltdown is currently considered one of nuclear power's most serious threats to public health. Fission product iodine is highly radioactive, it is concentrated by humans in the thyroid, and it has been assumed in the past that virtually all of it would be released to the atmosphere if fuel element-meltdown occurred.

Continuing thermodynamic studies under the BES program predicted that fission product iodine in light water nuclear reactor fuel rods should be chemically-bound as an iodide, probably cesium iodide, and not as molecular iodine as previously assumed. Stimulated by these studies, tests of irradiated commercial fuel rods were carried out under Nuclear Regulatory Commission sponsorship and the prediction based on the thermodynamics studies was verified.

The prediction, now bolstered by direct experiment, is in accord with the behavior of the reactor at Three Mile Island, where the observed release of iodine was only about one millionth of that expected. This work substantially improves our capability to predict the consequences of reactor accidents and could have a major impact on nuclear plant siting criteria and accident response procedures.

(Oak Ridge National Laboratory, T. B. Lindemer, E. C. Beahm and T. M. Besmann)

2. Dual-Phase Steels for Energy Efficient Cars

Reduction in the weight of new automobiles is providing a major contribution towards reduced fuel consumption per mile driven. Safety considerations however call for maintaining adequate strength and fracture resistance in the automobile structure. The strength and fracture resistance of steels depend on the structure and distribution of the phases of iron present -- in this case, ferrite and martensite. The composition of these phases in steel was studied using advanced electron microscopy capabilities uniquely available at LBL, making it possible to optimize the structure of steel for strength and fracture resistance. As a result, a new class of steel alloys which has greater strength and fracture resistance per unit weight than steels currently in use, has been designed. These steel alloys, called "dual-phase," can be fabricated using current commercial methods.

The annual energy savings possible through weight reduction by using these dual-phase steels in cars, trucks and trains may approach 10% of the 20 quads currently consumed by the transportation sector.

(Lawrence Berkeley Laboratory, G. Thomas)

3. Titanium Diboride Coating for Erosion Resistance

An extremely hard, wear-resistant titanium diboride coating for use on materials that must survive extremely erosive environments has been developed under a project to study the basic mechanisms of fracture and erosion in various chemical and thermal environments and to determine techniques to minimize failure.

Titanium diboride may have many applications where wear-resistant materials are needed. It is difficult to fabricate in bulk form, but coatings of the material can be readily deposited on surfaces by means of chemical vapor deposition techniques. The coatings exhibit excellent erosion resistance.

Initial laboratory tests of titanium diboride applications have focused on its use as a coating for coal liquefaction reactor letdown valves. Erosion of these valves has long been a limiting factor in the life of coal liquefaction processing systems. A new composite valve with the tip coated with approximately a 50 micron thickness of titanium diboride has been undergoing tests.

Two prototype valves, used as the primary and secondary letdown valve pair in a continuous flow reactor, have been opened and shut 1300 times with little degradation. Untreated stainless steel valves used in the same way eroded and failed after 30 opening and closing operations. The new valves are scheduled for tests at a pilot coal liquefaction plant. The uses of titanium diboride coatings for fusion reactor applications and as coatings on cathodes used in the electrolytic reduction of aluminum are also being studied.

(Sandia National Laboratory, E. Randich)

4. Layered Ultra-Thin Coherent Structures to Produce New Properties

Superconducting materials have been created in which as many as one-half of the atoms were normally non-superconducting copper. These materials are composed of layers only a few atoms thick, of different atoms which normally do not combine in a coherent fashion. Research on the synthesis of layered materials has shown that as the layer thicknesses are reduced and approach single atom thickness, the properties of the composite change dramatically. For example, an assembly of alternate layers of niobium with copper behaved as a homogeneous superconductor although half of the layers were of normally non-superconducting copper. This technique for synthesizing ultra-thin coherent structures offers the possibility of creating entirely new materials with predetemined properties.

(Argonne National Laboratory, I. Schuller, C. Falco)

5. Non-Destructive Evaluation of Oil-Bearing Shales

Small angle neutron and x-ray scattering techniques have been applied in a nondestructive way to determine the size, shape and amount of oil bearing pores in oil shale. Using neutrons from the Hign Flux Isotope Reactor, information on the total pore distribution was obtained by small angle scattering of the neutrons. X-ray small angle scattering was used on the same sample to determine the pore distribution for empty pores. The difference between the two sets of data provides information on oil bearing pores. This technique demonstrates the capability to obtain highly complex information on a material accurately and quickly. In the case of oil shale, the information obtained is important in determining not only the oil content but the choice of initial and secondary recovery methods.

(Oak Ridge National Laboratory, G. Wignall, H. R. Child)

6. Superconducting Device Used to Search for Geothermal Fields

A device known as the SQUID (Superconducting Quantum Interference Device), capable of detecting very small changes in the earth's magnetic field has been built in a portable form. The changes in the earth's magnetic field that are detectable are in a range that may be due to the presence of water or oil and the SQUID is being used in field studies. Recent measurements in Mexico in a known geothermal field have revealed a likely potential for extensive new geothermal sources along a fault line. Mexico plans to drill in this area for confirmation. The application of this device to search for geothermal fields resulted from research dealing with quantum theory and experiments related to it. The extreme resolution of the SQUID apparatus permits measurements at the limit of current theory and may lead to further refinement or verification of quantum theory as it is understood today.

(Lawrence Berkeley Laboratory, J. Clarke)

7. Kinetics of Hydrogen Permeation in Metals

The properties of many materials are strongly affected by hydrogen on their surfaces or diffusing into them. Recent experiments have led to a quantitative understanding of the rate at which hydrogen is dissolved in metals. It has been demonstrated that thin layers of palladium on niobium metal dramatically increased hydrogen adsorption, with the significant result that every hydrogen molecule impinging on the surface splits into separate hydrogen atoms. The experimental results correspond to the surface reaction steps of adsorption and dissociation being two hundred times greater on a palladium coated niobium surface than on clean uncoated niobium, and a similar enhancement of the permeation of the hydrogen atoms through the niobium. This work is expected to provide guidance for new catalyst development where an increase of one or two hundred in hydrogenation catalyst reactivity would constitute a breakthrough. In addition, this research will impact on hydrogen storage technologies, in which rapid hydrogen permeation into and out of materials is desirable, yet limited by surface reactions.

(Brookhaven National Laboratory, J. Davenport, G. Dienes, M. Pick, M. Strongin)

8. Increased Photovoltaic Efficiency of Silicon Hydrides

A method has been developed to control the di- and tri-hydride content in amorphous silicon hydride for increased photovoltaic efficiency. The defect structure of silicon and the nature of the alloyed hydrogen determine the alloy's optical and electrical behavior which in turn governs its photovoltaic efficiency. It has been found that initial introduction of hydrogen into the amorphous silicon matrix forms a silicon monohydride which has a good photovoltaic response.

As more hydrogen is added, however, di- and tri-hydrides form which degrade the photovoltaic properties. Recent results have shown that the additional implantation of other elements (e.g. helium) can displace the hydrogen from the dihydride configuration to the monohydride defect, thus opening the possibility of tailoring alloys for optimum properties.

(Pacific Northwest Laboratory, Pawlewicz; Sandia National Laboratory, H. J. Stein)

9. New Class of Cryogenic Steels

Research aimed at understanding brittle fracture paths in steels and at developing alloying and heat treatments to avoid these paths has led to a new and promising class of cryogenic alloys. These have been found to have sufficient strength, fracture resistance, and formability for applications such as for pressure vessels to contain liquid natural gas, or for support structures for superconducting magnets. The alloys are ferritic steels containing manganese, but no nickel. This result may also have wide-ranging implications for the control of intergranular failure in other steels damaged by improper heat treatments.

(Lawrence Berkeley Laboratory, J. Morris)

10. Cyclic Irradiation Enhanced Deformation

Radiation damage to structural materials in both fission and fusion environments continues to be an important research area. The ability to predict such damage and its effects after long periods of service is critical. The development of techniques to stimulate this damage in a controlled way to better understand the mechanisms involved is a goal of the research program. The phenomenon of "creep", deformation of the fuel rod cladding, observed with reactor structural materials exposed simultaneously to radiation and stress at high temperature, is being examined with ion simulation techniques. It was found that the creep phenomenon is greater per unit of radiation received under cycling conditions -- bursts of radiation interspersed with low exposure periods -- than under steady conditions. A mechanism has been postulated to explain this phenomenon and is being tested. This insight is expected to find early use in both nuclear and fusion reactor design and development activities.

(Pacific Northwest Laboratory, E. P. Simonen)

11. Plutonium Specific Complexing Agent Synthesized

A new class of chelating (from Greek for "claw") agents has been synthesized, one of which has been found to remove plutonium selectively from animal tissues. This class of chemical compounds has been designed on a molecular scale to satisfy two criteria crucial to precise selectivity: geometric configuration to fit that of the plutonium species to be removed, and a chemical bonding match to a plutonium ion bearing a plus four charge. The immediate interest has been in the application of the newly synthesized LICAM-C (linear catechoylamide carboxylate) to living systems where it was shown that, with minimal side effects, one dose of LICAM-C removed, through the kidneys, 70% of the plutonium injected into mice. This work has attracted attention in the public press, and LICAM-C has received publicity as a potential decontaminating agent in the case of accidents involving uptake of plutonium by people. Less dramatic, but of perhaps greater significance, is the possibility of tailoring chemical extractants to treat both nuclear and chemical wastes for removal of noxious species and recovery of valuable materials from dilute sources.

(Lawrence Berkeley Laboratory, K. Raymond, F. Weitl)

12. Water Photolysis Process Yielding Hydrogen and a Stable Oxygen Species

A photolytic process yielding gaseous hydrogen and trapping the active oxygen simultaneously produced in a stable form of probable interest for industrial application has been discovered. Photolytic reactions induced by sunlight in water normally yield atomic hydrogen and oxygen-containing species such as the hydroxyl radical. The hydrogen atoms produced combine to form gaseous molecular hydrogen, but if the oxygen-containing species is not readily removed from the system, or if it does not readily react to produce gaseous oxygen, the production of hydrogen will soon terminate. In water splitting as in many other chemical reactions, the inability to remove a product from a reacting system often results in the buildup of species that initiate undesirable reverse or side reactions in the system. What has been discovered is a reacting system that overcomes this difficulty -- i.e., the oxygen-containing species is not a problem but a desirable product -- and should permit the development of a continuous photolytic process yielding hydrogen and usefully combined oxygen.

(Lawrence Berkeley Laboratory, M. Calvin)

13. Catalyst Regeneration for Coal Gasification

Research has provided new insight into the poisoning by sulfur of the metal catalysts used for the methanation step of coal gasification. With this new insight also has come the demonstration that poisoned catalysts can be regenerated far more completely than current practice achieves. This may significantly improve economics of these catalyst systems for coal processing by extending the useful life of the catalysts and increasing the plant operating factor.

The usual regeneration practice for removal of the chemisorbed sulfur has been to heat the catalyst in air in order to oxidize the sulfur to gaseous sulfur dioxide. Since the catalyst surface also becomes oxidized and catalytically inactivated, normal practice has been to follow up with a hydrogen treatment which removes the oxygen. With the air treatment, however, an undesired oxidation of the metal surface proceeds faster than the desired oxidation of sulfur, which results in "buried" sulfur under the newly formed layers of metal oxide. The competing oxidation rates can be manipulated to favor oxidation of sulfur over that of metal, by drastically lowering the oxygen concentration to 1-10 parts per million and by carefully controlling the temperature. The catalyst, regenerated in this way, regains nearly 100 per cent of its original activity. The concept may be applicable to other catalytic systems which are poisoned by sulfur.

(University of Delaware, J. Katzer)

14. Catalyst Using Synthesis Gas as a Reducing Agent

Molecular hydrogen is required in many chemical processes involving reactions carried out through catalysis. However, the production of large quantities of chemically pure hydrogen is energy-consuming and expensive. A homogeneous rhodium carbonyl catalyst system which allows direct utilization of synthesis gas (mixture of CO and H_2) as a reducing reagent in place of molecular hydrogen for a specific class of reactions has been discovered. Synthesis gas is the principal product of the gasification of coal or char; it is a mixture of carbon monoxide and hydrogen of widely varying composition depending on the conditions used. Current practice requires further processing and separations to obtain hydrogen for use as a reducing agent. The catalytic reduction discovered proceeds by consuming both the CO and H_2 in proportion to their initial concentrations, thus allowing for the direct utilization of any composition of synthesis gas. The catalytic reduction reactions found are applicable in a number of industrial processes including production of plastics and some of the manmade fibers.

(University of Texas, R. Pettit)

15. Production of Highly Charged Ions for Fusion-Related Research

The study of highly charged ions -- atoms which have been stripped of most of their electrons -- is important to development of fusion energy because these ions may occur in fusion plasmas and dramatically reduce their energy. Until now obtaining such highly stripped ions for laboratory research on their properties was possible only in energy ranges far above those typical of fusion plasmas. A new method has been devised which overcomes this problem. It involves a beam of particles at millions of electron volts striking a gas target and stripping the gas molecules of most of their electrons. The resulting highly charged ions emerge from the target at relatively low energies, only a few tens of electron volts, an energy range heretofore not attainable for such highly charged ions. The ions are then accelerated to a few hundred electron volts for the fusion-related experiments. This technique is being adopted by several laboratories.

(Kansas State University, P. Richard, L. Cocke)

16. Sulfur Dioxide and Nitrogen Oxides Effect on Atmospheric Levels of Carbon Monoxide

Recent measurements of the isotopic (oxygen-18/oxygen-16) ratio in atmospheric carbon monoxide (CO) indicate a relatively large increase of technologically produced CO during this past 8 years. This increase, from 1971 to 1979, is by an amount greater than that attributable to the largest sources of technological CO, the internal combustion engine (ICE). Two possible explanations are: (1) a large increase from biomass burning which produces CO difficult to distinguish from ICE carbon monoxide or (2) a decrease in the atmospheric concentration of hydroxyl free radicals (OH) which are the principal scavengers of CO from the atmosphere. The first explanation does not seem very likely since patterns of biomass combustion have not changed dramatically during the past 10 years. The second possibility is disturbing, particularly if the reduction of OH radicals in the atmosphere were caused by an increase in the pollutant trace-gas scavengers for OH, such as sulfur dioxide and the nitrogen oxides.

(Argonne National Laboratory, C. Stevens)

17. Palladium from Nuclear Waste

A technology for recovery of stable palladium during the reprocessing of nuclear fuel elements has been devised. Its implementation could ease our current heavy dependence on Soviet and South African palladium for automobile exhaust cleanup catalysts, and possible future use as a coal conversion catalyst.

The crux of the process is a strongly radiation-resistant system which enables the processing of spent nuclear fuel after a minimum of cooling time. The object is to remove fission product ruthenium as soon as possible. This ruthenium has a relatively short half-life of about one year, decaying into 30-second rhodium which decays to stable palladium-106. The required radiation-resistant system involves a high temperature chemical partitioning between molten uranium and magnesium. In this system, the required initial separation of ruthenium from the also-present radioactive palladium, with a separation factor greater than ten thousand, has been demonstrated. The stable palladium-106 is ultimately recovered free of radioactivity.

The U.S. production of palladium has never exceeded 1,000 kg per year while the consumption has reached 46,000 kg/yr. It is estimated that an annual production of about 1,000 kg is possible from reactors now operating or under construction.

(Oak Ridge National Laboratory, M. Duffie)

18. Energy Efficiency in Natural Systems Leads to New Thermodynamic Insight

Research on the mechanism of an important biochemical process has provided new thermodynamic insight into the possibility of attaining greater efficiency of energy utilization in complex chemical systems.

Living systems derive their energy supply from the conversion of ATP (adenosine triphosphate) to ADP (adenosine diphosphate). ADP is converted back to ATP during glycolysis, the process which converts sugars to oxidized chemicals via a multi-step (9 or more) reaction pathway. The concentrations of the intermediates in the glycolysis process are observed to oscillate, with frequencies on the order of 1 minute, with definite relationships among the different intermediates' concentrations and their frequencies.

A description of the thermodynamics of reactions in systems where intermediate species concentrations oscillate has been developed. It demonstrates that oscillations in the multi-step glycolysis sequence result in an increase of 10-15% in overall efficiency over that which would otherwise be observed. Essentially, this comes about because some of the energy which would be dissipated as heat is intercepted at peaks in the oscillations, and appears as useful chemical energy. Although developed to explain the biochemical phenomenon observed, the description has been recast to provide additional insight into the thermodynamics of a heat (Stirling) engine as an example of the generality of this concept.

(Stanford University, J. Ross)

19. Fluoroxysulfates: Powerful New Oxidants and Fluorinating Agents

A group of powerful oxidants and fluorinating agents which may prove to be uniquely useful synthetic and analytical tools for both inorganic and organic chemistry has been prepared, isolated and characterized. These are the first known ionic hypofluorites, or specifically, in this case, fluoroxysulfate (SO_4F^-) salts. The ionic character of these salts contribute to their relative stability. It is this stability and the ease of formation of these salts which make this new kind of reagent so potentially attractive. The fluoroxysulfate salt of rubidium or cesium separates out as a solid when fluorine gas is passed through a water solution of rubidium or cesium sulfate. Earlier, other chemists had noted that passing fluorine through aqueous sulfate solutions gave a powerful oxidant which decomposed in a few hours, but this observation had been largely ignored and even questioned before this recent work.

(Argonne National Laboratory, E. Appelman)

20. New Analytical Technique Using Fiber Optics Devised

A novel application for fiber optics may soon find many uses. A linear array has been assembled of 30 fibers (the number could be greater) with lengths varying from 1 to 59 meters, all leading into a single photomultiplier, a device which measures intensities of pulses of light. The 2 meter increment in length from one fiber to the next provides an incremental time delay of 10 nanoseconds (billionths of a second) between the pulses received by the photomultiplier from each fiber. A nanosecond pulse of light is spread by a diffraction grating into 30 different wavelength groups and each of these is focused on the receiving end of one of the 30 optical fibers. These all lead to the single photomultiplier, so that its output is a series of 30 electrical pulses, 10 nanoseconds apart, with intensity corresponding to the intensity of the light within the wavelength range of each fiber's placement.

The system can be tailor-made to monitor, as a function of time, the particular spectral range of interest in specific analytical applications. In practice it would compare a blank with a sample interposed between the light source and the diffraction grating, thus providing a fast, accurate analytical reading.

(Oak Ridge National Laboratory, H. Ross)

21. New Technique for Ohmic Contact Fabrication

During 1980, a project originally sponsored by Advanced Energy Projects (AEP), was found sufficiently promising to "graduate" from the program and receive favorable consideration for possible funding under DOE's Solar Technology Program. The project involved development of a technique called "arc plasma spraying," and also illustrates how the AEP program helps promote innovation: A small business firm -- four full-time and five part-time employees - received its first contract ever from AEP to develop a new method of fabricating ohmic contacts for solar cells. Assessment of the "arc plasma spraying" method shows it to be extremely well suited for mass production of large area solar cells.

(Solamat, Inc., J. Loferski, B. Roessler)

22. Powerful XUV Radiation Source Tunable at 83 nm Demonstrated

This project represents one of five different approaches to the development of new, bright and coherent X and XUV sources now under study. Such sources, when developed, will find applications in fusion plasma diagnostics, catalytic surface research, X-ray lithography, biology, medical diagnostics (X-ray holography) -- to name a few. This research has led to the development of the brightest laboratory radiation source ever observed in the soft X-ray region. The radiation, at 83 nm (nanometers, or 10-7 centimeters), is generated by using the third harmonic of tunable KrF* radiation in xenon. The radiation is coherent and tunable from 82.8 to 83.2 nm. At 83 nm, its spectral brightness is two orders of magnitude greater than that of the DORIS synchrotron, one of the brightest sources now operating.

There is now a reasonable possibility that in certain narrow wavelength regions, laser sources will compete with synchrotron light sources in brightness, at a small fraction of the cost.

(University of Illinois at Chicago Circle, C. Rhodes)

23. Novel Design for Solar Collectors

A new design for solar collectors allows increased separation between reflector and absorber surfaces. The novel approach for design of trough-like solar collector structures mitigates an important engineering limitation encountered in past design of such collectors, namely the requirement for very close spacing between the absorber and the reflector. In principle the effective absorbance of the structure as a whole drops sharply as the spacing increases. Yet some minimum spacing is required to allow a convection-reducing vacuum envelope to be placed around the absorber. The new design calls for corrugating a part of the surface of the reflector in a very specific but easily fabricable way. As a result, the optimum location of the absorber is shifted to a distance of up to one radius of the absorber which is ample for engineering purposes and does not degrade the collector performance.

(University of Chicago, R. Winston)

24. Fundamental Advances in Theory of Fluid Turbulence

The fine-scale motion of turbulent fluids plays a crucial role in many processes involving mass and energy transport. During 1980, scientists advanced a mathematical theory of fluid turbulence which enhances our ability to analyze the spatial, momentum and energy dynamics of rapidly moving fluids, such as may be found in heat exchangers, combustors and other devices important in energy transfer. The fine-scale motion of turbulent fluids (of the order of millimeters or less) is of concern also in practical design applications because of the vibrations and noise generated in turbulent flow. This theory, with its improved mathematical insights, is expected to find applications in design of more efficient, longer lasting components of energy systems.

(City University of New York, B. Levich)

25. Computational Method for Faster Energy System Modeling

Improving energy systems often depends on precise computation of system behavior. The same types of computation arise repeatedly throughout the energy field, and a major advance was made under our applied mathematical sciences program this year in handling one of the most important types -- called sparse least squares problems. More effective and realistic models will now be possible in analyzing, for example, structural integrity of fusion reactors and the efficiency of combustion processes. The advance came from new ideas on how to break down into simpler pieces the huge arrays of numbers that arise in these computations, and also on how to make optimum use of auxiliary computer storage, while avoiding the numerical instabilities that plague current methods. The new ideas have been incorporated into carefully constructed computer codes available to scientists and engineers throughout the nation.

(Oak Ridge National Laboratory, M. T. Heath; Stanford University, G. H. Golub)

26. Volcanic Gases Used to Fix Rock Histories

A mathematical code has been developed which effectively predicts the composition of gases from thermodynamics considerations in complex mixed systems at high temperatures. The code was developed to interpret volcanic gas compositions and tie them back to the energetics of the systems producing them and to provide information on the geologic history of these systems. Understanding the energy related aspects of volcanism is of particular importance in evaluating possible schemes for energy extraction from magma, and more generally, in gaining clearer insight into eruptive processes.

A valuable spin off of this work has been the use of this code to establish conditions required for controlled deposition from the gas phase of titanium boride, a process to provide a tough coating resistant to erosion prevalent in coal conversion applications.

(Sandia National Laboratory, A. T. Gerlach)

27. Mount St. Helens Yields Data on Particle Disperson, Magma Chambers

The eruptions of Mount St. Helens provided a unique opportunity for several DOE geoscience research programs. Preliminary results of experimenters concerned with volcanic gases at Sandia National Laboratory show that the volatile contents responsible for explosive eruptions may be relatively low. Volatile content has a large effect on magma viscosity and the recently acquired knowledge will be broadly useful in interpreting the geology of regions affected by recent or ancient volcanic activity. Other geosciences activities obtaining valuable information as a result of the Mount St. Helens eruptions include infrared photography and high altitude ash collection by Los Alamos Scientific Laboratory and analysis of data on atmospheric transparency changes on a continental scale by Pacific Northwest Laboratory. These activities are of value to the DOE long-range studies of climatic change.

28. Plant Polysaccharides as Hormones

Recently, it has been discovered that small polysaccharides (chains of sugars) act as regulators of plant growth and plant defense against attack by disease organisms. Plant-disease-causing fungi and bacteria produce specific small polysaccharides that act as hormones (messengers) causing the plant to produce new antibiotics, protective enzymes, and new growth blocking enemy attack. In addition, injury or trauma to plant cells causes release of specific enzymes that, in turn, release short polysaccharides from the plant's own cell wall. These cause specific changes in the plant depending on the type of "hormone" released. The data supports a novel hypothesis: The specificity of plant growth and response to disease relies upon a set of polysaccharide hormone-messengers. This new knowledge will add significantly to our ability to program plants for improved biomass production.

(University of Colorado, P. Albersheim)

29. Microbial Production of Hydrocarbons

Micro-organisms have been isolated that are capable of synthesizing, from simple carbon compounds, hydrocarbons with a chemical compositional pattern resembling that found in petroleum. Some of these micro-organisms can produce sizable amounts of hydrocarbons; however, these organisms are slow growing. The discovery of the existence of organisms with this capability suggests that others with similar properties, but with more advantageous growth rates, might also be found or genetically tailored.

(Colorado State University, T. Tornabene)

30. Anti-Flowering Compounds in Plants

Anti-flowering substances in plants have been discovered. Until now the prevailing concept has been that flowering occurs when a flowering hormone acts to initiate the process. More recently the presence of anti-flowering substances which can be transmitted through grafts has been shown. This advance sheds light on the chemical control over flowering and bears on biomass productivity since flowering can significantly reduce biomass production.

(Michigan State University, A. Lang)

13. **What level of General Plant Projects (GPP) and General Purpose Equipment (GPE) funding has each of the DOE laboratories received and is expected to receive for the period FY 1981 - FY 1985?**

    Answer: The following table identifies the amount of GPP funds provided to the laboratories for the period FY 1981 - FY 1985 and identifies the program providing the funds:

GPP FUNDING BY LABORATORY BY PROGRAM
($ in Thousands)
B/A

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Ames					
Basic Energy Sciences Program.................	$ 300	$ 300	$ 275	$ 275	$ 600

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Argonne					
Breeder Program..........	2,300	3,400	500	1,600	0
Basic Energy Sciences Program...............	0[a]	0[a]	0[a]	0[a]	5,000
	2,300	3,400	500	1,600	5,000
Brookhaven					
High Energy Physics Program.................	2,600	2,900	3,000	3,200	5,700
Idaho National Engineering Laboratory					
Defense Waste Program....	1,800	3,500	2,935	4,400	6,455
Lawrence Berkeley Laboratory					
Nuclear Physics Program..	2,100	1,500	1,500	1,500	2,500
Lawrence Livermore National Laboratory					
Weapons Activities Program.................	4,200	4,500	4,000	6,000	8,800
Materials Production Program.................	500	300	1,100	2,000	0
Biological & Environmental Research Program........	300	300	340	210	250
Magnetic Fusion Program..	0	0	1,080	1,000	1,000
Advanced Isotope Separation Program................	600	100	200	400	500
	5,600	5,200	6,720	9,610	10,550
Oak Ridge					
Magnetic Fusion Program..	3,300	4,300	3,500	4,200	7,000
Defense Waste Program....	1,000	800	2,000	1,870	2,500
	4,300	5,100	5,500	6,070	9,500
HEDL					
Nuclear Waste Tech Program.................	1,500	1,100	1,000	1,400	1,000
Breeder Program..........	2,700	2,800	1,500	1,900	4,900
	4,200	3,900	2,500	3,300	5,900
Pacific Northwest Laboratory					
Biological & Environmental Research Program....	0[b]	0[b]	1,100[b]	1,400[b]	2,000
Sandia National Laboratory					
Weapons Activities Program.................	2,800	4,400	4,000	5,000	7,500
Basic Energy Sciences Program.................	0	0	0	100	0
	2,800	4,400	4,000	5,100	7,500

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Savannah River					
Materials Production Program..................	2,200	2,400	2,714	3,133	3,900
Biological & Environmental Research Program.........	0	0	50	50	50
Defense Waste Program....	200	100	500	1,740	1,970
	2,400	2,500	3,264	4,923	5,920
LASL					
Weapons Activities Program.................	4,300	4,700	4,000	4,350	7,800
Materials Production Program.................	200	600	0	900	0
Defense Waste Program....	200	500	300	400	300
Nuclear Physics Program..	400	400	200	500	950
Biological & Environmental Research Program........	300	500	350	200	250
Magnetic Fusion Program..	0	0	420	300	300
Advanced Isotopes Separation Program......	300	100	0	0	0
	5,700	6,800	5,270	6,650	9,600

[a] Prior to FY 1985, the BES program did not have "landlord" responsibility for ANL

[b] Prior to FY 1985, the BER program did not have "landlord" responsibility for PNL.

The Office of the Controller does not have estimates available of GPE provided to the DOE laboratories so a complete GPE picture is not presented below. However, the following table identifies GPE funds provided to the laboratories by Office of Energy Research Program only. Data for FY 1981 was not available so we have displayed data for FY 1982 through FY 1985 only.

GPE FUNDING BY LABORATORY
Office of Energy Research Programs Only
($ In Thousands)
B/A

	FY 1982	FY 1983	FY 1984	FY 1985
Basic Energy Sciences Program				
Ames Laboratory	$ 140	$ 130	$ 140	$ 160
Argonne National Laboratory......	0[a]	0[a]	0[a]	2,000
Magnetic Fusion Program				
Oak Ridge National Laboratory....	3,260	4,000	4,000	3,600
High Energy Physics Program				
Brookhaven National Laboratory...	2,900	3,500	3,500	3,900

	FY 1982	FY 1983	FY 1984	FY 1985
Nuclear Physics Program				
Lawrence Berkeley Laboratory.....	800	800	800	800
Biological & Environmental Research Programs				
Oak Ridge Associated Universities	20	24	30	40
Pacific Northwest Laboratory.....	0[b]	1,200[b]	600[b]	0

[a] Prior to FY 1985, the BES program did not have "landlord" responsibility for ANL.

[b] The BER program did not have "landlord" responsibility for PNL prior to FY 1985.

14. Which DOE programs/subprograms fund GPP and GPE at each of the DOE laboratories?

Answer: The following table identifies the programs which provide GPP funds and GPE funds to the laboratories:

PROGRAMS WHICH SUPPORT GPP AT THE LABORATORIES

Ames
- Basic Energy Sciences Program

Argonne
- Breeder Program
- Basic Energy Sciences Program*

Brookhaven
- High Energy Physics Program

Idaho National Engineering Laboratory
- Defense Waste Program

Lawrence Berkely Laboratory
- Nuclear Physics Program

Lawrence Livermore National Laboratory
- Weapons Activities Program
- Materials Production Program
- Biological and Environmental Research Program
- Magnetic Fusion Program
- Advanced Isotope Separation Program

Oak Ridge
- Magnetic Fusion Program
- Defense Waste Program

HEDL
- Nuclear Waste Tech. Program
- Breeder Program

Pacific Northwest Laboratory
  Biological and Environmental Research

Sandia National Laboratory
  Weapons Activities Program
  Basic Energy Sciences Program

Savannah River
  Materials Production Program
  Biological and Environmental Research Program
  Defense Waste Program

LASL
  Weapons Activities Program
  Materials Production Program
  Defense Waste Program
  Nuclear Physics Program
  Biological and Environmental Research Program
  Magnetic Fusion Program

* Prior to FY 1985, the BES program did not have "landlord" responsibility for ANL.

The Office of the Controller was unable to identify which DOE programs provide GPE support to the laboratories. However, the following table identifies which Office of Energy Research Program provide GPE to the laboratories.

ER PROGRAMS WHICH SUPPORT GPE AT THE LABORATORIES

Basic Energy Sciences Program
  Ames Laboratory
  Argonne National Laboratory*

Magnetic Fusion Program
  Oak Ridge National Laboratory

High Energy Physics Program
  Brookhaven National Laboratory

Nuclear Physics Program
  Lawrence Berkeley Laboratory

Biological and Environmental Research Program
  Oak Ridge Associated Universities
  Pacific Northwest Laboratory

* Prior to FY 1985 the BES program did not have "landlord" responsibility for ANL.

15. How is it decided which DOE program/subprogram funds the GPP and GPE at each DOE laboratory?

Answer: The predominant program at a particular site, i.e., the single program with the largest amount of funds devoted to that site, has traditionally been assigned the responsibility to fund GPP and GPE at that site. The predominant program is then referred to as the "landlord" program for that site. An exception to this policy applies to the weapons laboratories where the defense program, although predominant in terms of funding support, only provides for defense program related GPP and GPE. Non-defense related GPP at the weapon laboratories is provided by the appropriate non-defense programs.

It is important to note that predominant program does not mean predominant organization. For example, a particular Assistant Secretary may provide cumulative support, from many programs, to a site which exceeds another Assistant Secretary's cumulative support. However, if the latter provides the greatest funding in a single program, that program becomes the "landlord" for the entire site.

16. How are the GPP and GPE funding priorities established? What criteria are used?

Answer: While the level of funds budgeted for GPP/GPE is determined by DOE Headquarters, the field offices determine priorities for use of these funds based on general site needs as well as programmatic needs. The GPP data sheets identify samples of projects that will be supported. Generally, GPP and GPE funds are used for the most urgent projects at the time the funds are actually available to the field offices.

GPP projects are intended to be utilized for construction projects totalling less than $1,000,000. During preparation of the FY 1985 budget, the Laboratory Management Council directed that higher funding levels be requested for GPP/GPE in an attempt to maintain the DOE's physical plant assets and to start reversing the current trend of deteriorating facilities. GPE funds are used for equipment of a general site support nature such as fork lifts, lawn mowers, etc.

17. What criteria are used to determine whether or not a given project is to be funded by (a) GPP, (b) the Multiprogram General Purpose Facilities (MGPF) Program, or (c) the In-House Energy Management Program?

Answer: The MGPF program funds only line-item sized projects (ie.. those above $1 million) that benefit two or more programs where no one program uses more than 60% of the facility involved. GPP funds can support any general plant projects with the TEC's less than $1 million. The In-House Energy Management (IHEM) program funds both line-item and GPP sized projects; however, these projects must meet strict payback requirements based on energy cost savings. Payback is only one factor among many considered in the MGPF and GPP programs. Others include safety, health, environment, security, as well as programmatic need and impact.

In general the MGPF program rehabilitates or replaces "multiprogram" facilities when they are deteriorated or constitute a hazard to personnel, operations or other facilities; whereas the IHEM program could replace a given facility if it meets their cost payback criteria (usually 3-5 years) GPP funding levels are established in Headquarters, but, the actual projects undertaken are determined in the field based on a process which determines the highest priority current need each has developed.

18. What centralized management does DOE provide in general, and BES in particular, for the (a) GPP, (b) MPGF Program, and (c) the In-House Energy Management Program?

Answer: All budgets are reviewed in terms of overall levels, issues and interactions at the Assistant Secretary level via the Internal Review Budget and the Institutional Planning processes. The MGPF and IHEM Programs operate agency-wide and their staffs coordinate their budget requests and activities continuously. The IHEM is managed by the Office of Project and Facilities Management, under the Assistant Secretary, Management and Administration. The MGPF Program is managed for the DOE by the Office of Field Operations Management under the Director, Office of Energy Research. The staff a) provides overall program and budget review, b) delegates project execution responsibilities to the Operation's Office and reviews performance periodically, c) does on-site reviews, and d) requests periodic reporting.

The GPP budget is also reviewed on both a Departmental wide basis and also by each of the program offices responsible for managing specific GPP requirements. On a department wide basis GPP levels are reviewed by the Assistant Secretary for Management and Administration. After the program level the GPP requests are reviewed on a more detailed basis both during the formulation and execution phase for each of the projects supported.

19. What block funding does DOE award in general, and BES in particular, to universities? Which universities have been funded and are expected to be funded by this method for the period FY 1981 - FY 1985?

Answer: The BES program does not award block grants to universities. The grants made available to universities are for specific research proposals which have been reviewed on a case by case basis and which fit with the mission requirements of the Department and program.

20. How much has the BES Program contributed to the support of DOE's Small Business Innovative Research (SBIR) Program for FY 1983? How much is estimated for FY 1984 and FY 1985? How was this assessment determined?

Answer: The BES Program contributed $537,000 to the SBIR program in FY 1983 and we estimate that $1,740,000 and $3,445,000 will be contributed in FY 1984 and FY 1985, respectively. The assessment was based on the amount of extramural research conducted by the BES Program and was applied by year according to the percentages persuant to the SBIR.

A. Holifield Tables

1. The January 31, 1984 "Holifield Tables" indicate that the IRB Fiscal Year 1985 budget request for the Basic Energy Sciences (BES) program totalled $418,440,000, including $347,085,000 for operating expenses and $71,355,000 for PACE. According to these Tables, the Department's FY 1985 submission to OMB for the program totalled $407,250,000, including $333,410,000 for operating expenses and $73,840,000 for PACE. What are the specific differences between these two budgets?

Answer: Please see the table below and explanation that follows for the differences between the FY 1985 IRB and the FY 1985 OMB Budget.

(Dollars in thousands)

	FY 1985 IRB Request	FY 1985 OMB Request	Change
Basic Energy Sciences (BES)*			
Materials Sciences			
Operating Expenses.................	$147,210	$140,710	$- 6,500
Capital Equipment..................	15,950	15,450	- 500
Construction.......................	36,000	35,100	- 900
Subtotal...........................	199,160	191,260	- 7,900
Chemical Sciences			
Operating Expenses.................	83,680	85,630	+ 1,950
Capital Equipment..................	7,140	8,840	+ 1,700
Construction.......................	4,900	8,050	+ 3,150
Subtotal...........................	95,720	102,520	+ 6,800
Nuclear Sciences			
Operating Expenses.................	55,155	50,185	- 4,970
Capital Equipment..................	3,620	2,950	- 670
Construction.......................	600	300	- 300
Subtotal...........................	59,375	53,435	- 5,940
Engineering and Geosciences			
Operating Expenses.................	29,000	26,975	- 2,025
Capital Equipment..................	1,825	2,000	+ 175
Subtotal...........................	30,825	28,975	- 1,850
Advanced Energy Projects			
Operating Expenses.................	12,280	10,910	- 1,370
Capital Equipment..................	320	320	0
Subtotal...........................	12,600	11,230	- 1,370
Biological Energy Research			
Operating Expenses.................	14,960	14,800	- 160
Capital Equipment..................	1,000	830	- 170
Subtotal...........................	15,960	15,630	- 330
Program Direction			
Operating Expenses.................	4,800	4,200	- 600
Subtotal...........................	4,800	4,200	- 600
Total			
Operating Expenses.................	347,085	333,410	-13,675
Capital Equipment..................	29,855	30,390	+ 535
Construction.......................	41,500	43,450	+ 1,950
Basic Energy Sciences..............	418,440	407,250	-11,190

* It should be noted that the Applied Mathematical Sciences subprogram was proposed as a separate program, called Energy Science Computational Research (ESCR), with a budget request of $54,145,000, during the OMB budget cycle. It was only after the OMB submission that the decision was made to include this program in Basic Energy Sciences budget.

Explanation of Budget Changes

General

- Budget changes principally the result of meeting OMB target levels. By subprogram the OMB budget reflects the following changes:

Materials Sciences

- A deferral of several new research thrusts
- A general reduction in the Advanced Materials Research Initiative

Chemical Sciences

- The addition of a new initiative in organic chemistry
- The added responsibility for GPE and GPP at Argonne National Laboratory

Nuclear Sciences

- The deferral of the Combustion Research Facility, Phase II
- A general reduction in the activities making up the Nuclear Sciences subprogram, including Nuclear Data, Heavy Ion Fusion, SSRL, Heavy Element Chemistry, and stable and special isotope Production

Engineering and Geosciences

- A deferral of several new research thrusts in Engineering and Geosciences (in computer aided engineering, and Continental Scientific Drilling)

Advanced Energy Projects

- A reduction in the number of projects supported by the subprogram

Biological Energy Research

- A modest share of the general reduction

Program Direction

- A reduction in the staffing level

2. As noted in question 1 above, the Holifield Tables indicated that the OMB FY 1985 budget request for the BES program totalled $407,250,000, including $333,410,000 for operating expenses and $73,840,000 for PACE. The FY 1985 Congressional request for BES totalled $419,530,000, including $348,340,000 for operating expenses and $71,190,000 for PACE. What are the specific differences between these two budgets?

Answer: Please see the table below and explanation that follows for the differences between the FY 1985 OMB Budget and the FY 1985 Congressional Budget.

(Dollars in thousands)

	FY 1985 OMB Request	FY 1985 Cong. Request	Change
Basic Energy Sciences			
Materials Sciences			
Operating Expenses.................	$140,710	$141,480	$+ 770
Capital Equipment..................	15,450	15,450	0
Construction.......................	35,100	31,720	-3,380
Subtotal...........................	191,260	188,650	- 2,610
Chemical Sciences			
Operating Expenses.................	85,630	80,930	- 4,700
Capital Equipment..................	8,840	8,840	0
Construction.......................	8,050	8,050	0
Subtotal...........................	102,520	97,820	- 4,700
Nuclear Sciences			
Operating Expenses.................	50,185	49,755	- 430
Capital Equipment..................	2,950	2,950	0
Construction.......................	300	300	0
Subtotal...........................	53,435	53,005	- 430
Applied Mathematical Sciences			
Operating Expenses.................	0	28,250	+28,250
Capital Equipment..................	0	1,500	+ 1,500
Subtotal...........................	0	29,750	+29,750
Engineering and Geosciences			
Operating Expenses.................	26,975	20,795	- 6,180
Capital Equipment..................	2,000	1,500	- 500
Subtotal...........................	28,975	22,295	- 6,680
Advanced Energy Projects			
Operating Expenses.................	10,910	10,810	- 100
Capital Equipment..................	320	320	0
Subtotal...........................	11,230	11,130	- 100
Biological Energy Research			
Operating Expenses.................	14,800	12,490	- 2,310
Capital Equipment..................	830	560	- 270
Subtotal...........................	15,630	13,050	- 2,580
Program Direction			
Operating Expenses.................	4,200	3,830	- 370
Subtotal...........................	4,200	3,830	- 370
Total			
Operating Expenses.................	333,410	348,340	+14,930
Capital Equipment..................	30,390	31,120	+ 730
Construction.......................	43,450	40,070	- 3,380
Basic Energy Sciences..............	407,250	419,530	+12,280

Explanation of Budget Change

General

- Budget changes were principally the result of meeting Administration budget targets. By subprogram the Congressional Budget request reflects the following changes:

Materials Sciences

- Prorata share of the management initiative savings
- No allocation for the Experimental Beam Halls at LANL
- No allocation for funding for the Advanced Light Source at LBL.
- Additional funds made available for research at SSRL.

Chemical Sciences

- The deferral of the new research thrust in catalysis and organic chemistry
- A prorata share of the management initiative savings

Nuclear Sciences

- A prorata share of the management initiative savings

Applied Mathematical Sciences

- The shift of the Energy Science Computational Research program to the BES budget.

Engineering and Geosciences

- The deferral of the enhanced research proposed in Continental Scientific Drilling and organic geochemistry
- No allocation for new research thrusts in Mechanical Sciences, Systems Sciences and Engineering Data and Analysis

Advanced Energy Projects

- A minor share of the management initiative savings

Biological Energy Research

- No allocation for the enhanced program proposed.

Program Direction

- Management initiative savings and reduction in staffing levels

3. **Given the information in questions 1 and 2 above, what are the specific differences between the Department's FY 1985 IRB and Congressional Request budgets for BES?**

Answer: Please see table below and explanation that follows for the differences between the FY 1985 IRB and the FY 1985 Congressional Budget.

(Dollars in thousands)

	FY 1985 IRB Request	FY 1985 Cong. Request	Change
Basic Energy Sciences (BES)			
Materials Sciences			
Operating Expenses..................	$147,210	$141,480	$- 5,730
Capital Equipment..................	15,950	15,450	- 500
Construction........................	36,000	31,720	- 4,280
Subtotal...........................	199,160	188,650	-10,510
Chemical Sciences			
Operating Expenses..................	83,680	80,930	- 2,750
Capital Equipment..................	7,140	8,840	+ 1,700
Construction........................	4,900	8,050	+ 3,150
Subtotal...........................	95,720	97,820	+ 2,100
Nuclear Sciences			
Operating Expenses..................	55,155	49,755	- 5,400
Capital Equipment..................	3,620	2,950	- 670
Construction........................	600	300	- 300
Subtotal...........................	59,375	53,005	- 6,370
Applied Mathematical Sciences			
Operating Expenses..................	0	28,250	+28,250
Capital Equipment..................	0	1,500	+ 1,500
Subtotal...........................	0	29,750	+29,750
Engineering and Geosciences			
Operating Expenses..................	29,000	20,795	- 8,205
Capital Equipment..................	1,825	1,500	- 325
Subtotal...........................	30,825	22,295	- 8,530
Advanced Energy Projects			
Operating Expenses..................	12,280	10,810	- 1,470
Capital Equipment..................	320	320	0
Subtotal...........................	12,600	11,130	- 1,470
Biological Energy Research			
Operating Expenses..................	14,960	12,490	- 2,470
Capital Equipment..................	1,000	560	- 440
Subtotal...........................	15,960	13,050	- 2,910
Program Direction			
Operating Expenses..................	4,800	3,830	- 970
Subtotal...........................	4,800	3,830	- 970
Total			
Operating Expenses..................	347,085	348,340	+ 1,255
Capital Equipment..................	29,855	31,120	+ 1,265
Construction........................	41,500	40,070	- 1,430
Basic Energy Sciences................	418,440	419,530	+ 1,090

Explanation of Budget Change

General

- The Congressional Budget reflects changes made to reflect Department and OMB priorities and the need to meet overall budget targets. The details by subprogram reflect a combination of the items discussed in detail in the previous Holifield Table answers. As indicated earlier the decision was made after the OMB Budget discussions to include the Energy Science Computational Research program in the BES budget and therefore not have this activity as a separate DOE program.

B. Management Initiatives

1. **According to the BES budget justification (Congressional Budget Request, FY 1985, Volume 3, p. 145), the FY 1985 budget request of $419,530,000 reflects $3,000,000 for savings resulting from management initiatives in the area of administrative processes/field structure. What specific initiatives will result in these savings?**

Answer: This management initiative is one of several initiatives which reflect the first implementation efforts of the DOE with regard to recommendations contained in various studies of departmental operations, including the President's Private Sector Survey on cost control (The Grace Commission) and the Federal Laboratory Panel of the White House Science Council (The Packard Report), as well as the Administration's program for improved management systems known as Reform 88.

The $3,000,000 in the BES program represents savings in FY 1985 resulting from improved management of government owned, contractor operated (GOCO) facilities. This initiative involves improved utilization of private sector business practices by GOCO contractors through reduced procedural controls and heightened reliance on policy issuances and performance evaluation by the DOE Operations Offices. Cost initiatives for improved GOCO performance and reduction in reporting detail will lead to DOE management oversight at a higher level and to improved opportunities for innovation and implementation of new management processes by GOCO contractors. These savings will occur at all eight DOE operations offices and major contractors.

2. **Who will determine how these specific initiatives result in these savings?**

Answer: These initiatives will involve a wide variety of activities including a thorough examination of reporting requirements and reductions in those requirements and a thorough examination of procedural requirements levied on our contractors in such areas of achievements as socioeconomic procurement goals, management of subcontractor activities, program and management planning activities and others. In each case the principal staff or program office responsible for the activity being examined will be required to identify savings opportunities and initiate the actions to implement those activities. For example: reduction in procurement reporting requirements would be directed by the Procurement Office, reduction in ADP reporting by the Office of ADP Management and so forth. The overall effort will be coordinated and results will be assessed by the Assistant Secretary for Management and Administration.

3. How will these savings be apportioned among the DOE Operations Offices, laboratories, and other contractors?

Answer: All field offices and GOCO contractors will be expected to contribute efforts to achieve these savings. The impact on any individual organization will depend upon our assessment of the collective affect of eliminating or consolidating reporting requirements or simplifying procedures. For example: If a particular organization has estimated that meeting a particular reporting requirement requires four staff years of effort and that requirement is eliminated, we would expect the organization in question could reduce their overhead staffing by four staff years. While the data for making these estimates are not precise we believe it is sufficient to arrive at a reasonable basis to allocate the resultant savings without adverse impact on programmatic activities.

C. BES Facilities/Collaborative Research Centers

GENERAL

1. For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, Accelerator and Reactor Improvement and Modification Projects, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to each facility supported totally or partially by the BES program, including the following: (i) Ames Laboratory Materials Preparation Center; (ii) Argonne National Laboratory (ANL) Atomic Spectroscopy Facility; (iii) ANL 4.5-MV Dynamitron Accelerator; (iv) ANL High Voltage Electron Microscope Tandem Facility; (v) ANL Intense Pulsed Neutron Source (IPNS-1); (vi) ANL Premium Coal Sample Program; (vii) ANL Pulse Radiolysis Facility; (viii) Brookhaven National Laboratory (BNL) High Flux Beam Reactor (HFBR); (ix) BNL National Synchrotron Light Source (NSLS); (x) Kansas State University James R. Macdonald Laboratory; (xi) Lawrence Berkeley Laboratory (LBL) National Center for Electron Microscopy; (xii) Los Alamos National Laboratory (LANL) Spallation Neutron Research/Proton Storage Ring (SNR/PSR) Facility; (xiii) Los Alamos Equation of State Library Center; (xiv) Notre Dame Radiation Laboratory (NDRL) Pulse Radiolysis Laboratory; (xv) NDRL Radioysis- ESR Facility; (xvi) Oak Ridge National Laboratory (ORNL) Electromagnetic Isotope Preparation Facility (Calutrons); (xvii) ORNL EN-Tandem Facility; (xviii) ORNL High Flux Isotope Reactor (HFIR); (xix) ORNL National Center for Small-Angle Scattering Research; (xx) Oak Ridge Electron Linear Accelerator (ORELA); (xxi) ORNL Shared Research Equipment Program (SHaRE); (xxii) ORNL Surface Modification and Characterization Laboratory; (xxiii) ORNL Transuranium Processing Plant (TRU); (xxiv) University Isotope Separator at Oak Ridge (UNISOR); (xxv) Sandia National Laboratories Combustion Research Facility (CRF); (xxvi) Stanford Synchrotron Radiation Laboratory (SSRL), (xxvii) Research Computer Facilities (RCF's); and (xxviii) any additional facilities not identified above. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Advanced Mathematical Sciences, any other BES subprograms, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, Fossil Energy, Conservation, etc.).

Answer: This question concerns 27 centers, facilities or groupings of major equipment that fall into three general categories: 1. User Facilities, 2. Imbedded Facilities -- major equipment or facilities which are part of a research program and are available on a limited basis outside the funded project, and 3. centers that are primarily operated to provide a service to the research community.

Thirteen of the facility/centers identified in the question fall into the first category. User facilities are those where facility operating support is provided separately from support for research utilization by the sponsoring DOE subprogram. In most cases, separate Field Task Proposals are submitted by the host laboratory to DOE for facility support. The following facilities fall into this category:

ANL:	High Voltage Electron Microscope Tandem Facility Intense Pulsed Neutron Source
BNL:	High Flux Beam Reactor National Synchrotron Light Source
LBL:	National Center for Electron Microscopy
LANL:	Spallation Neutron Research/Proton Storage Ring
ORNL:	High Flux Isotope Reactor National Center for Small Angle Scattering Research Oak Ridge Electron Linear Accelerator Shared Research Equipment Program Surface Modification and Characterization Laboratory
SNL-L:	Combustion Research Facility

Stanford Synchrotron Radiation Laboratory

For each of these, a table has been prepared for insertion into the record providing the detailed information requested. For the purposes of this question, we have used the following definitions:

Operations: This includes costs to operate the facility, providing services to users, whether included under the "in-house" or "out-of-house" definitions below, and other operating expenses identified below.

In-house research: Cost of in-house user research projects, including dedicated equipment. At the IPNS, for example, the support provided by the Materials Sciences subprogram for ANL staff carrying out research using the IPNS meets this definition.

Out-of-house research: Cost to support non-host laboratory researchers using a facility, including dedicated equipment. The source of support may be DOE, other federal agencies, industry, etc. In most cases it can only be estimated although the number of outside users can normally be identified.

Other operating expenses: These include spare parts, "changes in inventory" such as for nuclear reactor fuel elements, and similar items.

Capital equipment: Includes separately budgeted equipment funds provided by BES directly to the facility.

ARIM: Includes BES provided construction funds for accelerator reactor, improvement or modification.

GPP: Funds provided by the responsible program to the host laboratory for general plant projects which are directly related to the facility; BES does not have GPP (or GPE) budget responsibility for any of the laboratories identified in the first category except for ANL beginning in FY 1985.

In-house energy management: BES has no direct involvement in this item; any numbers provided were obtained as information from the laboratories.

(iv) Argonne National Laboratory High Voltage Electron Microscope Tandem Facility

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	560	550	615	685	750
In-house research	BES/MS	600	750	450	500	600
	OTHER	0	0	520E	780E	860E
Out-of-house research	BES/MS*	10	10	15	20	25
	DOE,OFA INDUSTRY, OTHER	500	650	750E	800E	1200E
Capital Equipment	BES/MS	370	35	235E	900E	925E
GPP	*	0	0	0	200	800

* Numbers provided by Laboratory
E = Laboratory estimate based on number of users and time allotted

II

(v) Argonne National Laboratory Intense Pulsed Neutron Source

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	4929	3685	3895	4712	5066
	INDUSTRY	0	0	0	17	30
In-House research	BES/MS	1410	1690	2200	2300	2400
Out-of-house research	BES/MS	0	0	400E	465E	540E
	DOE/OTHER	N/A	350	252E	895E	982E
	INDUSTRY	N/A	125	125E	145E	170E
	OFA/NSF	N/A	350	400E	465E	540E
	UNIV.	N/A	575	600E	700E	815E
	FOREIGN	N/A	250	400E	465E	540E
Capital Equipment	BES/MS*	180	300	300	275	450
GPP	*	12	75	70	25	145

* Numbers provided by Laboratory
E = Laboratory estimate based on number of outside users and time at IPNS

III

(viii) Brookhaven National Laboratory High Flux Beam Reactor

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	4067	4700	6057	6600	7800
In-house research	BES/MS	2433	2630	2698	2900	3200
	BES/CS	666	722	410	420	455
	ER/NP	962	1135	1300	826	900
	ER/BER*	528	606	624	683	727
Out-of-house research	BES/MS	0	0	307E	330E	354E
	OFA	1039	1154	1268E	1363E	1464E
	NON FED	395	438	487E	523E	563E
Other operating expenses	BES/MS	47	301	200	433	1000
Capital Equipment	BES/MS	145	175	200	400	700
	BES/CS	50	175	50	60	60
	ER/NP	181	90	90	100	125
	ER/BER	150	150	141	32	69
ARIM		0	0	0	40	500
GPP	*	0	0	66	80	120
In-house energy management	*	0	0	285	0	0

* Numbers provided by Laboratory
E = Laboratory estimate based on number of outside users and time at HFBR

IV

(ix) Brookhaven National Laboratory National Synchrotron Light Source

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	2599	5098	5922	7795	8700
	BES/CS	0	2404	3800	4470	5600
In-house research	BES/MS	1390	1738	1604	1800	2100
	BES/CS	1009	1112	1570	1880	2030
	BES/AEP	136	165	104E	390E	90E
	ER/OTHER	0	0	493E	913E	1137E
Out-of-house research	ER/OTHER	0	0	1303E	2245E	2690E
	DOE/OTHER & OFA	1930	2315	1910E	2160E	2240E
	NON-FED	1225	1470	1980E	3225E	3960E
Other operating expenses	BES/MS	170	468	250	167	700
Capital Equipment	BES/MS	1047	1326	900	800	800
	BES/CS	288	729	770	790	340
	BES/AEP	0	0	0	160E	100E
	ER/OTHER	337	745	600E	240E	100E
ARIM		0	265	100E	600E	1100E
GPP		406	239	611E	475E	700E
In-house energy management	*	0	66	0	0	100E
Phase II construction	BES/MS	0	0	0	2500	10000

* Numbers provided by Laboratory
E = Laboratory estimate based on number of users and time allotted

V

(xi) LBL National Center for Electron Microscopy

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	505	767	880	1090	1490
In-house research	BES/MS	0	0	500	650	800
Out-of-house research	OTHER	0	0	500E	650E	800E
Capital Equipment		238	80	300	350	400
Other specific construction projects attributable to this facility		3152	1955	463E	270E	100E

E = Laboratory estimate based on number of outside users and time at NCEM

VI

(xii) Los Alamos National Laboratory Spallation Neutron Research/Proton Storage Ring (SNR/PSR)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	0	0	0	0	500
	DOE/DP*	1373	1578	1450	1600	1700
In-house research	BES/MS	819	1190	1530	1570	1800
	DOE/DP*	600	635	710	800	1165
Capital Equipment	BES/MS	130	250	250	300	600
	OTHER*	13	50	50	90	100
GPP	*	390	0	0	0	0
SNR Improvement project	BES/MS	0	0	2700	0	0

* Numbers provided by Laboratory

VII

(xviii) ORNL High Flux Isotope Reactor

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/NS	3494	3798	5590	6150	7820
	BES/MS	781	918	0	0	0
	DOE/NE	182	130	100	0	0
	ER/OFE	146	400	0	0	0
	ER/HER	182	200	0	0	0
(Rev. fm isotope sales)		779	842	644	805	726
(Rev. fm other, internal sources/services provided:		198	311	383	409	355

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
In-house research	BES/MS	1894	1602	1868E	2190E	2370E
	ER/OFE	1200	1350	1460E	1617E	1545E
	DOE/NE	800	650	583E	500E	600E
Out-of-house research	DOE, OFA, INDUSTRY, OTHER	600	700	950E	720E	1540E
	RES EQ*	0	0	679E	720E	0E
Other operating expenses	BES/NS	0	0	0	0	1450
Capital Equipment	BES/MS	82	170	200	400	600
	BES/NS	152	484	70	120	80
ARIM		0	0	0	0	300E
GPP		0	0	0	0	250E

* Includes specialized research equipment for use at HFIR and Japanese neutron diffractometer

E = Laboratory estimate based on number of outside users and time at HFIR

VIII

(xix) ORNL National Center for Small-Angle Scattering Research
(Center dependent on neutrons produced at HFIR)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	NSF*	463	486	472	466	625
In-house research	NSF*	88	95	91	89	142
	BES/MS*	100	100	90	90	100
Out-of-house research	DOE, OFA, OTHERS	1200	1200	800E	800E	1200E
Capital Equipment	NSF*	0	0	60	100	26
Other Construction		0	124	0	0	0

* Estimate by Laboratory of sources of in-house support from various projects

E = Laboratory estimate based on number of outside users and time using small angle scattering facility

IX

(xx) Oak Ridge Electron Linear Accelerator (ORELA)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/NS	1261	1443	1546	1600	1650
In-house research	BES/NS	947	1185	1363	1520	1765
	HENP/NP	609	553	50	50	50*
	OFA	28	27	37	38	32
	ER/OTHER	0	31	36	40	43
	DOE/NE	1008	980	856	756	200

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Capital Equipment	BES/NS	153	154	154	180	500
	HENP/NP	99	107	0	0	0
	DOE/NE	57	67	17	0	0
GPP	*	0	0	340	0	0

* Decrease because of reprogramming of funds to Holifield Facility

X

(xxi) ORNL Shared Research Equipment Program (SHaRE)

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	220	230	260	290	320
	BES/OTHER	40	45	50	55	58
In-house research*	BES/MS	900	1000	1292E	1680E	1930E
	ER/MFE	190	200	200E	220E	250E
	CONS	0	0	75E	80E	85E
	FOSSIL	20	30	50E	60E	70E
	NUCLEAR	200	150	100E	50E	50E
Out-of-house research	DOE, OFA, INDUSTRY, OTHER	810	1032	1047E	1137E	1195E
Capital Equipment	BES/MS	25	370	75E	290E	325E
	ER/FE	0	250	325E	0	0
	DOE/NE	0	50	0	0	0
ARIM		0	0	325E	0	0

* Estimate by Laboratory of sources of in house support from various projects
E = Laboratory estimate based on number of users and equipment used

XI

(xxii) ORNL Surface Modification and Characterization Laboratory

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/MS	0	0	460	500	850
In-house research	BES/MS	857	1283	1120	1220	1280
	ER/OFE	125E	195E	125E	125E	125E
	OTHER	0	0	50	0	0
Out-of-house research	DOE, OFA, INDUSTRY, OTHER	0	0	400E	400E	600E
Other Operating Expenses		70	0	0	200E	0
Capital Equipment		99	633	257E	595E	825E
GPP		0	235E	235E	650E	500E

E = Laboratory estimate based on number of outside users and time at SMCL

XII

(xxv) Sandia National Laboratories Combustion Research Facility

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations	BES/CS	1900	1930	2170	2490	2750
In-house research	BES/CS	1400	1840	2160	2290	2500
	BES/OTHER*	870	1020	1340	1450	1560
	DP*	0	0	500	750	1000
	CE*	1200	1350	1450	1650	1900
	OFA/NRC*	0	0	330	500	670
	FOSSIL*	1030	1650	1320	1400	1700
Out-of-house research	BES/CS*	300	480	680	730	770
	INDUSTRY	0	0	40E	20E	200E
Capital Equipment		800	975	900	800	700
GPP		0	0	0	100	530

* Numbers providad by Laboratory
E = Laboratory estimate based on number of outside users and time at CRF

XIII

(xxvi) Stanford Synchrotron Radiation Laboratory

	Support Source	FY 1981 (K$)	FY 1982 (K$)	FY 1983 (K$)	FY 1984 (K$)	FY 1985 (K$)
Operations**	BES/NS	***	***	6192	6577	7980
In-house research	BES/NS	0	0	152	159	0
	BES/MS	0	0	0	700	895
Out-of-house research	BES/NS	0	0	0	0	0
	OTHER*	0	0	21600E	3200E	42900E
Capital Equipment	BES/NS	0	0	456	490	600
	BES/MS	0	0	0	100	300
GPP		0	0	0	0	100
Other specific construction projects attributable to this facility		0	0	100E	2790E	10130E

*   Numbers provided by Laboratory
** Operated primarily as a user facility
*** Funded by NSF in 1981 and 1982
E = Laboratory estimate based on number of outside users, time on SSRL and time at home institutions devoted to preparing experiments, analyzing data

Eight of the facility/centers fall into the second category of "Imbedded Facilities". They involve specialized pieces of equipment which are central to, and part of, the conduct of a large research project. Their operating costs are usually not separately broken out but are included in the funds provided for the implementation of the research project employing them. The equipment/facility may be made available to qualified users on a case-by-case basis at no cost, when appropriate. The imbedded facility/centers are:

ANL Atomic Spectroscopy Facility
ANL 4.5-MV Dynamitron Accelerator
ANL Pulse Radiolysis Facility
Kansas State University James R. Macdonald Laboratory
Notre Dame Radiation Laboratory Pulse Radiolysis Facility
Notre Dame Radiation Laboratory Radiolysis ESR Facility
ORNL EN-Tandem Facility
Research Computer Facilities

The ANL 4.5 MV Dynamitron and the ANL Pulse Radiolysis Facilities are jointly funded by BES and HENP. Accelerator and Reactor Improvement and Modification funds have been provided to these facilities as follows ($K):

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
ANL 4.5 MV Dynamitron (Nuc. Physics)	0	0	300	100	0
ORNL EN-Tandem Facility	200	0	100	250	0

The Kansas State University James R. Macdonald Laboratory is a university-owned atomic physics facility. Research support provided by BES includes funding for operation of an accelerator. Included in the BES FY 1985 request are funds, $2 million, to initiate upgrading of the accelerator at a total estimated cost of $3.4 million to DOE ($1.4 million will be requested to complete the project in FY 1986). Additionally, the State of Kansas will provide $0.6 million to upgrade the housing for the accelerator.

There are 11 Research Computer Facilities, 10 at DOE laboratories and 1 at a university, each consisting of one or more minicomputers dedicated primarily to a specific thrust of the Applied Mathematical Sciences subprogram of BES Operation of the facilities is supported within the framework of each of the individual projects. Capital equipment funding for these facilities was $800,000 in FY 1983, $970,000 in FY 1984, and the FY 1985 request is for $1.5 million.

Five of the facility/centers fall into the third category. Service facilities generally do not have a research component directly at the facility except to improve the service provided, and operate on a subsidized or cost reimbursable basis. They are listed below and discussed separately.

Ames Laboratory Materials Preparation Center
ANL Premium Coal Sample Bank
LANL Equation of State Library
ORNL Electromagnetic Isotope Preparation Program
ORNL Transuranium Processing Plant

Ames Laboratory Materials Preparation Center
$K

	FY 1982	FY 1983	FY 1984	FY 1985
Operations - Total	366	892	950	1067
Ames Laboratory Orders	216	687	740	817
Non Ames Laboratory Orders	150	205	210	250

The facility started operating in FY 1982. It operates on a cost reimbursable basis and has no independent facility operating budget. The center consists of special sample preparation apparatus and personnel trained in its use. Samples which are not available from other sources are prepared on order according to specifications on a best effort basis. The center also provides analytical services and acts as a clearing house/referral system for information about the availability of special research samples

ANL Premium Coal Sample Program
$K

	FY 1983	FY 1984	FY 1985
Operating - Chemical Sciences	454	645	622

Funding for the ANL Premium Coal Sample Program was first provided in FY 1983. This program collects, prepares and distributes reference grade samples of a small number of representative coals for the use of qualified researchers to establish benchmark experimental measurements in coal science. Exceptionally uniform samples are specially prepared and stored in an inert atmosphere to ensure the chemical stability of the coal over a long period of time.

Los Alamos Equation of State Library
$K

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operating total	300	305	320	350	250
Operating BES-Materials Sciences	140	125	120	125	0
Other - Defense Programs	160	180	200	225	250(Est.)

This facility is a computer based Library of Equation of State data and FORTRAN subroutines developed at Los Alamos which are made available without charge to qualified scientists and engineers.

ORNL Electromagnetic Isotope Preparation Facility

$K

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operating total	2400	3615	3263	3580	5000
Facility	2180	3379	3013	3220	4630
R&D	220	236	250	360	370
Operating Source	2400	3615	3275	3580	5000
Isotope Sales	1380	2860	2205	2500	2700
OHER	0	0	250	400	600
BES - Nuclear Science	1020	755	820	680	1700
Capital Equipment					
BES - Nuclear Science	48	32	200	500	500
ARIM	0	0	0	270	0
GPP	0	0	0	0	100

This facility separates stable isotopes for the Research Materials Collection (non consumable).

ORNL Transuranium Processing Plant (TRU)

$K

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operating total	4953	5554	6173	6473	6799
Separations BES - Nuc. Sci.	3740	4200	4800	5136	5490
Process R&D (NE)	1095	1175	1148	1157	1167
Misc. Reimbursable Services	75	92	134	85	92
Capital Equipment BES - Nuc. Sci.	43	52	91	95	50
Nuclear Energy	0	35	0	0	0

This facility is used to perform two functions. Its principal use is the chemical separation of heavily irradiated target materials for the purpose of preparing research samples of the rare, highly radioactive transuranium elements, none of which occur in nature. A secondary effort is devoted to chemical separations process development funded by the Nuclear Energy program.

2. **How much funding has been provided by other federal agencies such as the National Science Foundation, by State agencies, or by other nations for each of the facilities enumerated in question 1 above?**

Answer: Funding provided by other federal agencies is discussed in the answers provided for each facility. A copy of this information is attached.

Ames Laboratory Materials Preparation Center

Budget Authority

Outside Sales of MPC (dollars in thousands)

	FY 1982	FY 1983	FY 1984	FY 1985
Federal Agencies	$ 86	$ 76	$ 99	$ 118
State Agencies	15	18	21	25
Foreign Institutions	13	48	34	40
Private Sources	36	63	56	67
	$150	$205	$210	$250

Argonne National Laboratory Atomic Spectroscopy Facility

None.

Argonne National Laboratory 4.5-MV Dynamitron Accelerator

There is no funding from other federal agencies, foreign institutions, or private sources.

Argonne National Laboratory High Voltage Electron Microscope Tandem Facility

None.

Argonne National Laboratory Intense Pulsed Neutron Source (IPNS-I)

There has been no funding for IPNS operation by any other federal or state agency, or foreign institution. However, in two important areas of technology transfer IPNS-related activities have been funded. First, the development and successful construction of an uranium target at IPNS led the Japanese to request (in early 1982) that ANL build one for them. This contract was signed in 1983, and the target is to be delivered in late 1984. The Japanese are paying in excess of $300,000 for this. Second, the successful operation of the world's first neutron position sensitive scintillator detector led the Institut Laue Langevin (Grenoble, France) to contract for such a detector, which will be delivered in early 1985. The charge for this by ANL is $80,000.

Argonne National Laboratory Premium Coal Sample Program

To date no funding has been received from sources other than the DOE. Funding from other sources may be provided by organizations which request the processing of additional coals on a cost reimbursement basis. An Australian group has expressed interest in processing up to 4 brown coals at a cost of about $40,000 each.

Argonne National Laboratory Pulse Radiolysis Facility

None.

Brookhaven National Laboratory High Flux Beam Reactor (HFBR)

B/A
($ in 000's)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
National Science Foundation	259	250	250	250	250
Exxon Corp. (Equip.)	0	0	500	0	0
U.S. - Japan Coop. Prog.	0	0	27	33	40
U.S. - Japan (Equip.)	0	300	400	200	0

Brookhaven National Laboratory National Synchrotron Light Source (NSLS)

Outside User Research*
B/A (Thousands)

	FY 1983	FY 1984	FY 1985
Other Federal Agencies (NSF, Commerce, NIH)	1080	1168	930
Industry	3195	980	800
State Agencies	110	60	60
Total	4385	2208	1790

* DOE: FY 1983 - $922; FY 1984 - $1,090; FY 1985 - $1,240.

Kansas State University James R. Macdonald Laboratory

KSU contributions to laboratory operations (in $1,000): (includes salaries and wages, plus benefits and indirect costs, and Nuclear Science Laboratory funds for periods corresponding to above contract years)

FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
156	230	194	209	226

Total: 1015

Lawrence Berkeley Laboratory National Center for Electron Microscopy

No money was provided for the facilities or operations by other agencies.

Los Alamos National Laboratory Spallation Neutron Research/Proton Storage Ring (SNR/PSR) Facility

None has been provided or expected from any of these sources.

Los Alamos National Laboratory Los Alamos Equation of State Library Center

No direct funding was provided by other federal agencies,

Notre Dame Radiation Laboratory Pulse Radiolysis Facility

No funding has been or is expected from other Federal agencies or private sources.

Notre Dame Radiation Laboratory Radiolysis-ESR Facility

No funding has been or is expected from other Federal agencies or private sources.

Oak Ridge National Laboratory Electromagnetic Isotope Preparation Facility (Calutrons)

No funds have been provided by other federal agencies, state agencies, foreign institutions, or private agencies.

Oak Ridge National Laboratory EN-Tandem Facility

The EN-Tandem has received no funding from other Federal agencies, State agencies, foreign institutions, or private sources.

Oak Ridge National Laboratory High Flux Isotope Reactor (HFIR)

Funding by other than DOE (Operating and Equipment):

		(Budget Authority in Thousands)			
	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
U.S.-Japan Program	0	$360	$360	$396	$220
The above amounts include equipment furnished by Japan amounting to:	0	(230)	(50)	(130)	0
U.S.-Japan Program in MFE*	0	0	0	0	476
Isotope Production**	781	918	644	805	726

* Under a U.S./Japan collaborative agreement, the Japanese funds will be received by DOE Headquarters and funded to ORNL as DOE programmatic funds.

Oak Ridge National Laboratory National Center For Small-Angle Scattering Research (NCSASR)

All direct funding for the NCSASR has been and is expected to be provided by the National Science Foundation. Contracts with several industrial organizations to carry out proprietary research on a cost recovery basis have been concluded. Some two thousand dollars have been paid into the Center from this source. It is expected that modest sums will continue to be realized from proprietary research.

All indirect funding (e.g. travel, living expenses, sample preparation, etc.) for users is furnished by the users' institutions or by grants from federal agencies to the users.

Oak Ridge National Laboratory Oak Ridge Electron Linear Accelerator (ORELA)

The Defense Nuclear Agency has been providing $30,000 per year for maintenance and upgrade of the Evaluated Nuclear Data File/Version B (ENDF/B) data files for which they have accepted responsibility.

Oak Ridge National Laboratory Shared Research Equipment Program (SHaRE)

No direct funds received or expected.

Oak Ridge National Laboratory
Surface Modification and Characterization Facility

The majority of all funding research programs comes from the Office of Basic Energy Sciences, Division of Materials Sciences, USDOE. Through FY 1983 only $50,000 was supplied by other federal agencies (U.S. Army) and $50,000 from private sources (industry). No significant change is anticipated through FY 1985. All indirect funding (e.g., travel, living expenses, sample preparation, etc.) for users is furnished by the users' institutions or by grants from federal agencies to the users.

Oak Ridge National Laboratory Transuranium Processing Plant (TRU)

Funding by other federal agencies and private sources has always been very small and arises in the form of payments for special services required for preparing, packaging, and handling certain research samples.

Sandia National Laboratories, Livermore Combustion Research Facility (CRF)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Nuclear Regulatory Commission	0	0	330	500	670
Industry Funds*	0	0	40	20	200

* Industry funding is from Motor Vehicles Manufacturers Association (MVMA) and Electric Power Research Institute (EPRI). The 200K in FY 1985 is total anticipated from EPRI and MVMA.

Stanford Linear Accelerator Center
Stanford Synchrotron Radiation Laboratory (SSRL)

(Budget Authority in Thousands)

	FY 1981*	FY 1982*	FY 1983	FY 1984	FY 1985
Other Federal Sources	5455	5394	635	467	467
Other Non-Federal Sources	117	134	198	138	150
	5572	5528	833	605	617
Construction					
Other Federal Sources	0	770	902	803	0
Other Non-Federal Sources	209	1430	916	475	0
	209	2200	1818	1278	0

* NSF provided the principal support for SSRL until FY 1983, when it was transferred to DOE.

University of Illinois at Urbana-Champaign
Center for Microanalysis of Materials

	1981	1982	1983	1984	1985
			(B/A in thousands)		
Other Govt. Agencies	178	314	507	450	415
Private Sources	22	23	24	30	35

Note. All dollar amounts are in thousands of dollars.

3. **What is the BES user policy for each of the facilities listed in question 1 above?**

Answer: The user policy for each of the facilities is discussed in the answers provided for each facility. A copy of this information is attached.

Ames Laboratory Materials Preparation Center

The policy of the MPC is that all the operations pertaining to the preparation, purification, and fabrication of pure materials are performed by Ames Laboratory personnel. Quantities of the ultrapure rare-earth and refractory metals and alloys in single and polycrystalline forms are available providing: (1) the material/service cannot be obtained from a commercial source and (2) that material will not be resold. Students and researchers are welcome to visit the center to learn specific operations on a prearranged basis.

Argonne National Laboratory Atomic Spectroscopy Facility

This facility, while not an official user facility, is open to all qualified users. Experiments by outside users are encouraged. Potential users arrange an experimental schedule which is appropriate for both the user and the in-house scientists. The majority of such experiments are collaborations with in-house scientists.

Argonne National Laboratory 4.5-MV Dynamitron Accelerator

The Dynamitron is not an official user facility; however, we accommodate outside users and we encourage the active collaboration of outside users in our in-house research programs. Projects suggested by outside users should be relevant to these programs and the results must be published in the open literature.

Argonne National Laboratory High Voltage Electron Microscope Tandem Facility

The Electron Microscopy Center for Materials Research has a well-defined user policy for the HVEM-Tandem Facility, which is the only unique national users facility currently available within the Center. (An appropriate user policy for the new advanced Analytical Electron Microscope will be developed within the next year in conjunction with the HVEM-Tandem Facility Steering Committee.) The user policy for the HVEM-Tandem Facility has been established by the management of the Materials Science and Technology (MST)

Division at ANL with advice from a HVEM-Tandem Facility Steering Committee made up of eight representatives from academic and industrial research institutions and seven ANL/MST research staff members. The chairperson of the Committee is elected annually by the members. The Steering Committee handles general matters of Facility development and evaluation of research proposals and use priorities for the Facility. Priority use of the Facility is for fundamental materials research that will be published in the open literature. All major use of the HVEM-Tandem Facility is obtained through research or technical proposals submitted to the Steering Committee. The criteria for evaluation of a proposal and the allotment of use time include scientific merit, feasibility, need for the use of these unique facilities, and compatibility of the proposed research with Facility equipment and operational priorities. In general, the Committee seeks to maintain an approximately 50% non-ANL usage of schedulable time. All users with approved research proposals have priority use of Facility equipment. Requests for minor use of the Facility may be discussed directly with the Facility manager. The provision for limited usage is intended to provide time for exploratory investigations.

Scientists from universities and government and industrial laboratories are invited to use the Electron Microscopy Center for Materials Research and its HVEM-Tandem Facility in furthering their research. However, any activity which can be carried out through commercially available laboratories, such as that which can be performed on the Center's more conventional microscopes, is not appropriate for this Center.

While there are no use charges for basic research, the users are responsible for all expenses associated with their research. Facility funds permit replacement of malfunctioning equipment subjected to normal use, but the cost of replacement of items damaged by a user because of negligent or improper operation may be levied against his research funds. Industrial users wishing to carry out proprietary research are charged for the use of the Facility. Users must give credit to the sponsoring agency (DOE/BES) of the Facility in all reports, publications and presentations arising from use of the Facility. Facility staff are available during one or two shifts a day to instruct experimenters in the use of the equipment, and in some instances to participate in experimental programs. Since Facility staff must maintain and upgrade the facility equipment. it is expected that researchers will become competent to operate the equipment without ANL assistance. To this end, a course of lectures on high-voltage electron microscopy has been given and is available on videotape together with supplemental lecture notes for potential users. Research proposals are normally accepted for eighteen months of work, but may be renewed. Sixteen months after the acceptance of a proposal, the authors should submit a report summarizing their work, together with copies of other reports and publications and a list of oral presentations. Proposals for modifications of the Facility systems must be submitted to the Steering Committee for approval and then scheduled by the manager. Equipment that is developed for use with the Facility through these projects shall in general become the property of the Facility after the first anniversary of its initial use. The user shall provide the Facility staff with adequate documentation to allow service and use of the equipment by other workers.

Argonne National Laboratory Intense Pulsed Neutron Source (IPNS-I)

The user policy at IPNS is well defined and has been successfully implemented since startup in November 1981. Twenty-five percent of the beam time for each instrument is assigned to the Argonne scientist responsible for that instrument. The remaining 75% of beam time is assigned by a Program Committee (joint with WNR/PSR at Los Alamos) based on proposals submitted twice a year. The Program Committee consists of thirteen scientists, two from ANL, two from LANL and nine from outside. The chairman is also from outside the DOE laboratories. Experimenters who are allocated beam time by the Program Committee have free use of the instruments, ancillary equipment (furnaces, cryostats, high-pressure cells, etc.), data acquisition system, and technical assistance. The central computer can be accessed free from the user's home institution for data analysis and refinement. Users from North American universities can receive full travel and living support from the University of Chicago, which has also provided a car for the users. Proprietary beam time can be purchased for $2400/instrument day (24 hours). Another important factor in the IPNS user policy has been the variety of schools, workshops, and conferences that we have sponsored to inform the outside scientific community about the scientific possibilities at IPNS. No less than eleven such functions have been held since 1981. A description of them is in the IPNS Progress Report. A total of 825 scientists have attended these functions.

Argonne National Laboratory Premium Coal Sample Program

The user policy has several elements. Samples will be made available to all qualified basic research people. A nominal charge will be made for samples to defray replacement cost over a period of time. Sample recipients will be asked to provide references to published reports and other publications which may result from research on supplied samples, so that they may be shared with the rest of the basic research community. The facility will be made available to external sponsors for the processing of suitable coals on a reimbursed cost basis. The same standards used for the collection, preparation and distribution of samples for the Premium Coal Sample Program will apply to any externally sponsored efforts. Work for external sponsors will be done subject to the schedule for the work sponsored by the U. S. Department of Energy.

Argonne National Laboratory Pulse Radiolysis Facility

The facility, though not a formally-designated user facility, is open to all qualified users, and experiments by outside users are encouraged. Potential users arrange an experimental schedule appropriate for the user and in-house scientists. The majority of such experiments are collaborations with in-house scientists.

Brookhaven National Laboratory High Flux Beam Reactor (HFBR)

The HFBR is a National User Facility; workers from other laboratories are able to carry out experiments there, after peer review of their research program. In the past, there have been different approaches to the implementation of this policy for the different scientific disciplines. Starting in FY 1984, the Participating Research Team (PRT) system has been adopted for the HFBR. This will provide a unified users policy for the HFBR and the NSLS, where the PRT system is already in effect.

Existing and future spectrometers will be constructed and/or operated by PRT's, organized by discipline, and consisting of members from Brookhaven, universities, industry and other government laboratories. The PRT's are given priority for up to 75% of their spectrometers' operational time. General users are scheduled for PRT spectrometers and for certain instruments designated as general user facilities.

Brookhaven National Laboratory National Synchrotron Light Source (NSLS)

The NSLS is a national user facility available without charge to users. Proprietary work can be done on a full cost recovery basis, with the option to retain title to inventions resulting from research at the NSLS.

There are several modes of use of experimental facilities. A large number of beam lines have been designed and constructed by the 29 Participating Research Teams (PRTs). PRTs are, for the most part, user groups from outside BNL with large, long-range programs which have been approved by the NSLS Program Advisory Committee. The PRTs are given priority for up to 75% of their beam line's operational time. General users, who may have a less substantial need for the use of the facility, are scheduled for both PRT beam lines and for lines built by NSLS for the general community.

Kansas State University James R. Macdonald Laboratory

Users are presently invited to participate on a collaborative basis with in-house personnel. The upgraded facility will be operated on an open-to-all scientific merit basis.

Lawrence Berkeley Laboratory National Center for Electron Microscopy

Any qualified electron microscopist who proves scientific validity of his experiment as well as the need for the unique instrumentation provided here may use the facility.

Los Alamos National Laboratory Spallation Neutron Research/Proton Storage Ring (SNR/PSR) Facility

The SNR/PSR is being developed as a national user facility for neutron scattering research. A formal proposal procedure has been developed for the use of neutron scattering instrumentation, with a nationally appointed Program Advisory Committee (PAC) in cooperation with the Argonne National Laboratory to review proposals. The PAC is expected to make its recommendations on the basis of scientific excellence and optimal use of SNR/PSR characteristics. The PAC allocates two-thirds of the available neutron scattering beam time at the SNR/PSR. One third of the beam time is reserved for Laboratory discretionary research, defense programs, and instrument development. The use of neutron scattering instrumentation is free of charge to outside experimenters with approved proposals. Laboratory, university, and industrial proposals are treated on an equal basis. Following DOE policy, proprietary experiments will be conducted on a full cost recovery basis.

Los Alamos National Laboratory Los Alamos Equation of State Library Center

The present policy is to furnish the data base to any user upon request. We only ask that they supply the blank computer types. Since we are losing our support, we are, for FY 1985, instituting a small fee to recover some of our expenses.

Notre Dame Radiation Laboratory Pulse Radiolysis Facility

The facility is open to external users for either independent or collaborative work. Collaboration of external users is encouraged.

Notre Dame Radiation Laboratory Radiolysis-ESR Facility

The facility is open to external users for either independent or collaborative work. Collaboration of external users is encouraged.

Oak Ridge National Laboratory EN-Tandem Facility

The EN-Tandem Facility is open to qualified users from Oak Ridge National Laboratory, universities, and industries. Beam time and the use of existing devices and instrumentation are free of charge. Experiments are approved on the basis of a "request for beam time," by a Program Advisory Committee (PAC). The PAC consists of four staff members from the Accelerator Atomic Physics and EN-Tandem Operations groups. If the fractional utilization of the available time increases, and/or the number of requests from outside users rises, we will restructure the PAC to include outside user members. The only exception to the free beam time rule is for industrial users who request time for experiments that are not of direct interest to the Accelerator Atomic Physics Program. For these users a cost recovery charge has been made. In the last five years less than one week of time has been requested by one industrial user and the charges were less than $5,000.

Oak Ridge National Laboratory High Flux Isotope Reactor (HFIR)

The neutron scattering facilities are available to all scientists from other scientific organizations on a no-charge basis for research that is published in the open literature. Proprietary research can be performed through appropriate arrangements at full cost recovery.

The irradiation programs sponsored by ER are given first priority for reactor usage. DOE programs other than ER are given second priority, followed by other government programs and non-government programs, respectively.

Oak Ridge National Laboratory
National Center For Small-Angle Scattering Research (NCSASR)

The NCSASR is a National user-oriented facility. All beam time on the 30-m instrument and about 1/3 of the time on the 10-m SANS and 10-m SAXS machines is assigned to users, external and internal.

Oak Ridge National Laboratory Oak Ridge Electron Linear Accelerator (ORELA)

The Oak Ridge Electron Linear Accelerator (ORELA) is listed by the laboratory as a "user facility" because it is available to users. However, the nature of research of ORELA, which normally involves a long time commitment for experiments and for analysis of detailed data, leads to the situation where essentially all users have collaborated with an ORNL researcher who is performing continuing work toward objectives similar to those of the outside user. For this reason, there is no committee of users that sets schedules or advises management on policy.

Potential users of ORELA are asked to discuss their interest with a staff member doing similar work. Usually, this contact is automatic and requests originate in this manner. If the Oak Ridge National laboratory (ORNL) staff member is interested in the project, mutually convenient plans are set, consistent with other scheduling needs for the facility. In most cases, the outside user employs the equipment and the analysis programs normally used by his host, at least for the initial stages of data analysis.

Any request quite different from on-going work would come through ORELA management. We would accommodate the request if feasible. On a few occasions, we have suggested another facility which could perform the work more economically, e.g., experiments that require direct use of electron beams. In at least one case, an outside group performed a series of experiments at ORELA with no local collaborator and only some interaction with ORELA management to facilitate the work of the group and to assure personnel safety.

Oak Ridge National Laboratory Shared Research Equipment Program (SHaRE)

Letter proposals briefly describing collaborative research are submitted to the SHaRE Executive Committee for consideration. Approval is based on scientific excellence, previous research record of the proposers, relevance to DOE needs, and budget considerations. Access by users not requesting support from the ORAU SHaRE Program has always been granted subject only to limitations imposed by availability of the in-house staff.

Oak Ridge National Laboratory Surface Modification and Characterization Facility

Because of the complex nature of the materials alteration and analysis capabilities of the SMAC facility it is difficult for uninitiated users to benefit from independent utilization of the facility. Consequently, the SMAC Collaborative Research Center operates primarily in a collaborative mode where outside researchers work with SMAC facility staff. This policy insures efficient and safe utilization of the facilities; enables outside users to benefit from the cumulative expertise of SMAC staff in solving their particular problem quickly; and results in rapid and realistic technology transfer by doing proof-of-principle experiments on each user's particular materials problem. In the past, outside users have been accommodated through informal contacts with members of the SMAC staff. However, a more formal policy, involving written proposals and a proposal review committee, has been established recently.

The SMAC CRC also has provisions for doing proprietary research on a full-cost-recovery basis.

Sandia National Laboratories, Livermore Combustion Research Facility (CRF)

Qualified scientists are encouraged to take advantage of the specialized resources available at CRF. Prospective participants should submit a brief proposal to the laboratory director. Criteria for selection include technical merit, the extent to which CRF facilities are utilized, overlap with DOE program objectives, and the availability of specific equipment. In general, the CRF will host visiting scientists to use the special-purpose lasers, work with resident staff, make use of computers and codes, and to set up experiments. Visitors pay for their own salary, travel, housing, meals, and other local expenses. Facility lasers, apparatus, technicians, instrumentation, computers, and the services of support groups are provided at no cost for research which is not proprietary. Research results from non-proprietary projects are expected to be published and disseminated. For scientists with active government contracts, support for CRF research often can be arranged on an informal basis with the contract manager. There are opportunities for faculty, post-doctoral scientists, and graduate students to obtain Sandia support for combustion-related research at the CRF. In specific instances, proprietary research can be carried out at the CRF. For this type of work, the DOE will be reimbursed on a full cost recovery basis for the use of all CRF resources. Details of a DOE Class Waiver for patent rights are available.

Stanford Linear Accelerator Center
Stanford Synchrotron Radiation Laboratory

SSRL is open to all users on the basis of scientific competition. There are no charges for the use of the experimental facilities, except for proprietary research. This policy was put in place in 1975 by agreement with the National Science Foundation, the agency then supporting operation of SSRL. The policy has been very productive of excellent scientific results and has contributed strongly to the United States' position of leadership in synchrotron radiation research.

University of Illinois at Urbana-Champaign
Center for Microanalysis of Materials

This facility is not a DOE owned facility. The Center for the Microanalysis of Materials operates within the structure of the Materials Research Laboratory under the direction of the Director of the MRL. The policies which govern its operation are set by the Facility Committee and are approved by the MRL Director. Since the Center operates primarily for the benefit of its users the policies which govern their access are kept simple and are flexible.

The present policies may be summarized as follows:

a) Use of the facility requires approval of the Facility Committee which has delegated its authority of approval to the operational director of the laboratory in routine cases. Non-routine cases are referred to the Facility Committee for decision.

b) Access to the instruments requires that the user demonstrate competence in using the equipment. In the event that such competence does not exist, instruction in the use of the equipment can be arranged.

c) Scheduling of time on the instruments is arranged by the section leaders in the Center. In the case of any disputes these will be brought to the Facility Committee for adjudication.

d) Access to the facility for non-MRL users is arranged by the operational director of the lab on the basis of discussions with the prospective users. When possible, interactive research cooperation between the outside users and the facility personnel will be offered.

e) Use of the facility by non-MRL non-DOE users is restricted to projects which have a research component. Routine analysis which could be carried out by commercial facilities are not allowed.

f) All users are required to pay a fee the magnitude of which depends on the instrument used and the organization to which the user belongs and the source of research support. The magnitude of the fee is determined by the requirement that the operating costs of the instruments be recovered from the fees.

g) In the event that a prospective user has a meritorious project but cannot pay the user fee, he may petition the Facility Committee which has the authority to assign free time on the instrument. The intent of this policy is to prevent the application of the fee from interfering with the use of the instruments for desirable research applications.

4. **For the period FY 1981 - FY 1985, by facility and by user, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?**

Answer: The amount of reimbursable research is discussed in the answers provided for each facility. A copy of this information is attached.

Ames Laboratory Materials Preparation Center

(B/A in thousands)

	FY 1982 (beginning of MPC)	FY 1983	FY 1984	FY 1985
Reimbursable Research (Outside of House Laboratory Sales)	$150	$205	$210	$250

Argonne National Laboratory Atomic Spectroscopy Facility

None.

Argonne National Laboratory 4.5-MV Dynamitron Accelerator

None.

Argonne National Laboratory
High Voltage Electron Microscope Tandem Facility

During the period FY 1981 to the present no reimbursable research has taken place at the Facility. It is anticipated that very limited reimbursable research will take place at the Facility through FY 1985. Such research is planned by Shell Oil Co. should amount to about $2000 (i.e., 16 hours at $125 per hour) during the remainder of FY 1984. A similar amount within a factor of three might be anticipated for FY 1985.

Argonne National Laboratory Intense Pulsed Neutron Source (IPNS-I)

(Budget Authority in Thousands of Dollars)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Reimbursable Work	0	0	0	17*	30**

* Schlumberger-Doll Research

** Schlumberger-Doll work will continue. Also, contract negotiations are in progress with three other industrial laboratories. This number is a lower limit.

Argonne National Laboratory Premium Coal Sample Program

(Budget Authority in Thousands of Dollars)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Reimbursable Research	0	0	0	0	$160*

* Revenue for the processing of four Australian coals

Argonne National Laboratory Pulse Radiolysis Facility

(Budget Authority in Thousands of Dollars)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Reimbursable Research	0	0	17*	0	0

* Lawrence Livermore National Laboratory

Brookhaven National Laboratory High Flux Beam Reactor (HFBR)

For the five year period very little reimbursable work has been done at the HFBR. The work that has been performed was for irradiations with a value of less than $20,000 per year.

Brookhaven National Laboratory National Synchrotron Light Source (NSLS)

Estimates for reimbursible research are not available since arrangements are currently under negotiation with the companies involved. We roughly estimate $30,000 revenue from them in FY 1984 and $80,000 in FY 1985.

Kansas State University James R. Macdonald Laboratory

None in both cases.

Lawrence Berkeley Laboratory National Center for Electron Microscopy

Users are not charged for the use of the NCEM facility unless experiments involve proprietary data requiring confidentiality. The only reimbursable research during this period was done by Mobil Oil Company, 10 hour in January 1984 reimbursing the facility in the amount of $2,310. We do not foresee any further reimbursable research in the near future.

Los Alamos National Laboratory Spallation Neutron Research/Proton Storage Ring (SNR/PSR) Facility

None has taken place.

Notre Dame Radiation Laboratory Pulse Radiolysis Facility

None.

Notre Dame Radiation Laboratory Radiolysis-ESR Facility

None.

Oak Ridge National Laboratory EN-Tandem Facility

None.

Oak Ridge National Laboratory High Flux Isotope Reactor (HFIR)

None for neutron scattering.

Oak Ridge National Laboratory
National Center For Small-Angle Scattering Research (NCSASR)

Contracts for the accomplishment of proprietary research have been negotiated with du Pont, Firestone, and Eastman Kodak. Costs are assessed on a full-cost recovery basis. About $2000.00 has been received from this source. Modest use of this option is anticipated for the balance of 1984 and for 1985.

Oak Ridge National Laboratory Oak Ridge Electron Linear Accelerator (ORELA)

The only reimbursable research that has taken place at the Oak Ridge Electron Linear Accelerator during this period has been done for the Defense Nuclear Agency.

Defense Nuclear Agency Reimbursables
(dollars in thousands)

FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
$ 28	$ 27	$ 37	$ 38	$ 32

Oak Ridge National Laboratory Shared Research Equipment Program (SHaRE)

$147,000. One project from each Westinghouse-Bettis and the Air Force Weapons Laboratory. Both required ORNL staff participation.

Oak Ridge National Laboratory
Surface Modification and Characterization Facility

The SMAC facility began operation as a true users' facility only in FY 1984, although extensive collaborative research occurred prior to that on an informal basis.

Sandia National Laboratories, Livermore Combustion Research Facility (CRF)

No reimbursable work has been done at the Combustion Research Facility.

Stanford Linear Accelerator Center
Stanford Synchrotron Radiation Laboratory (SSRL)

The only research performed at SSRL which is reimbursable is proprietary. In the period FY 1981 to present, no reimbursable research was performed. It is anticipated that proprietary research will be done at the facility in the remainder of 1984 and in 1985. Revenues from this reimbursable research are estimated to be $3,000 in 1984 and $5,000 in 1985.

University of Illinois at Urbana-Champaign
Center for Microanalysis of Materials

In accord with the operating policy of the Center all research use of the facilities is on a reimbursable basis. The contract or organization which supports the research is asked to pay the usage fee which varies according to the instrument used. These fees are set at a level to meet the operating costs of the instruments.

Approximately 20% of the usage of the Center is by non-MRL programs which may be from other University of Illinois contracts, other University contracts, from Federally supported research facilities or from industrial firms. A partial listing of these outside users for a six month period is given below.

Northwestern University (B. Wessels, DOE) Radiation damage and native defect properties in zinc selenide.

Northwestern University (B. Wessels, NSF) Defects in indium phosphide.

American Philips Research (A. E. Morgan) Dopant segregation coefficients at the Si/SiO_2 interface.

Arizona State University (I.S.T. Tsong, DOE) Ion sputtering yields of Si and N.

Lawrence Livermore (C. Price, DOE) N2 diffusion profiles in steels and vanadium.

Crane Naval Labs (D. File) Photocathode defects.

U. S. Army ERADCOM (J. Oberstar) Penetration of contact elements. Diffusion of Be implants in doped InP.

Oxford University (C. J. Humphreys) Radiation damage in the beta-aluminas.

Sandia National Labs (B. Tuttle) Intergranular phases in ZnO varisters.

Oak Ridge National Laboratory (J.H. Schneibel) Sulphur Precipitation in Ni-Cr alloys.

Argonne National Laboratoy (J. Routbort) Oxygen diffusion in transition metal oxides.

University of Michigan, Ann Arbor (L.F. Allard, DOE) Microstructure of binder phases in ceramic interfaces.

Michigan State (Dr. Subramanian) Composition variation in spinodal decomposition.

Texas A&M University (J. Bockris) Structure of platinum deposits on semiconductors.

Argonne National Laboratory (R. Averbach) Ion beam mixing and enhanced diffusion.

California Institute of Technology (M. A. Nicolet) Influence of ion-implanted F and Cl on Si expitaxial re-growth.

American Philips Research (M.E. Lunnon) Rapid annealing of Boron implants in silicon.

EG and G (Idaho Falls) Preferred orientation in welds in stainless steels.

Cummins Engine Co. (G.L. Starr) Structures of ceramic coatings on metals.

1.0 Ames Laboratory Materials Preparation Center

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

   Answer: The Materials Preparation Center (MPC) was established to provide high purity metals and alloys for research. Within the research section of the Center, improvements in the metallurgical processing of refractory and rare-earth metals and alloys are being studied. Examples include: (1) new processes for preparing high purity transition metals, (2) technology for forming high strength Cu-Nb, Cu-Ta, Cu-Mo alloys that also have high electrical and thermal conductivities, and (3) establishing parameters for single crystal growth of pure metals, intermetallic compounds, solid solution alloys, and other materials.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

   Answer: The unique facilities of the MPC include: (1) ion exchange separation of the rare earth metals, (2) hydrofluorination of rare earth oxides, (3) preparation of ultrapure rare earth metals, (4) preparation of metals by thermite reduction, (5) electrotransport purification, (6) removal of carbon, nitrogen and oxygen from metals by external gettering, (7) electron-beam melting into platelet form, (8) preparation of ultrapure alkaline-earth metals, (9) precise analysis by scanning laser mass spectrometry.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

   Answer: The MPC has equipment and unique facilities for the preparation, purification, and fabrication of high purity rare-earth, refractory, alkaline-earth, and a few of the actinide metals. The various unit operations that are performed routinely by the MPC include: (1) ion-exchange separation of the rare-earth metals, (2) hydrofluorination, (3) preparation of sulfides, (4) metallothermic and thermite reductions, (5) non-consumable arc casting of metals, consumable arc casting, (6) induction heating and casting, (7) electron-beam melting, (8) high temperature sintering and hot pressing, (9) refining of metals by closed-crucible zone melting, (10) external gettering, and (11) electrotransport.

   Single crystals are prepared by: (1) arc-zone melting, (2) horizontal levitation zone melting, (3) cyclic temperature techniques, (4) float-zone melting, (5) recrystallization grain growth, and (6) Czochralski and Bridgman methods. Highly sinterable oxide powders are also prepared as well as many novel materials. The capabilities of these facilities are such that kilogram quantities of ultra-high purity materials can be prepared, purified, and fabricated into shapes essential to many basic science studies.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer:

1. Terfenol alloy ($Tb_{0.27}Dy_{0.73}Fe_{1.90-1.95}$) developed by the MPC in the past 2 years is a positive magnetostrictive material which vastly improves the performance of acoustic transducers. For high performances, it is essential that the elements which comprise this alloy are of high purity and that the grains are properly oriented by the directional solidification process. This material is of interest for underwater sonar devices, underground sonar for oil exploration, for micropositioning of instrument parts, for fuel injection systems, and for servo valves

2. Small amounts of the rare earth metals have been used as analytical standards.

3. In FY 1982, 4.7 kg of $PrNi_5$ prepared by the MPC was supplied to the University of Tokyo and was used in an adiabatic nuclear demagnetization refrigerator to achieve the lowest temperature ever attained, 27 microdegrees kelvin. This could not have been possible without the $PrNi_5$ compound being of exceptional purity

4. The Supercon Corporation, under a small business research grant, has used a Cu-18% Nb alloy to prepare a copper wire which has a yield strength of 320 ksi (much higher than stainless steel) and an electrical conductivity which is 67% of Cu. This alloy was prepared by the MPC and opened up the development of a new class of alloys that have high strength and good thermal and electrical conductivities.

In FY 1984 and FY 1985, additional high purity rare earth, refractory, and alkaline-earth metals will be prepared for various studies in national laboratories, universities and industrial laboratories. The transfer of the technology for preparing the terfenol alloys and possibly the copper-base refractory alloys to industry will begin so that these materials can be produced in large quantities by industry for our national defense and energy needs.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: In FY 1982, the MPC consisted of only the materials preparation section. In FY 1983, the analytical services section and the materials referral system and hotline were added. In FY 1984, the research section was added. The capital facility changes since the beginning of the MPC in FY 1982 have included high capacity rod rollers prepared from alloy steel, a 14 kW ultra-high vacuum (4×10^{-12} Torr) electron-beam zone melting furnace for preparing 1 cm diameter single crystals of Nb, Mo, Ta and W, a high capacity electrotransport unit capable of processing rods measuring 30 cm x 1 cm x 0.3 cm under pressures of $< 5 \times 10^{-11}$ Torr, a non-consumable arc furnace in which skull melts can be made and cast into chilled molds in a non-contaminating environment, and larger capacity for processing terfenol alloys by directional solidification. A new inductively-coupled plasma facility is planned which will be used to study the preparation of high melting refractory oxides and other materials.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer:

B/A ($ in thousands)

	FY 1982 (beginning of MPC)	FY 1983	FY 1984	FY 1985
Operations	0	0	0	0
In-House Research				
Material Sciences	$216	$602*	$678**	$745
Chemical Sciences	0	18	9	8
Fossil	0	67	53	55
Out-of-House Research	150	205	210	250
Capital Equipment	20	50	20	25
General Plants Project	0	0	0	0
In-House Energy Management	0	0	0	0

* Analytical services section and materials referral system (1/2 year) became operational.

** Research section initiated.

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer:

Budget Authority

	FY 1982	FY 1983	FY 1984	FY 1985
Federal Agencies	$ 86	$ 76	$ 99	$ 118
State Agencies	15	18	21	25
Foreign Institutions	13	48	34	40
Private Sources	36	63	56	67
	$150	$205	$210	$250

8. **For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.**

Answer:

	FY 1982*	FY 1983	FY 1984	FY 1985
FTE	4.6	11.1	12.2	13.4

* Beginning of MPC

9. What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?

Answer: The facilities of the MPC are utilized 100% of the time. A continuous backlog of requests exist and personnel are used to their maximum. Most of the equipment is in good condition and is essential to our preparation, purification, fabrication, and single crystal preparation efforts.

10. For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?

Answer: The MPC does not perform experiments, as such, but does make preparations and performs services for many investigators inside and outside the Ames Laboratory. These efforts for FY 1982, FY 1983, and projections for FY 1984 and FY 1985 are as follows:

Number of Preparations and Services

	FY 1982	FY 1983	FY 1984	FY 1985
In-House	140	170	200	230
Out-of-House	102	122	140	160

11. What is this facility's user policy?

Answer: The policy of the MPC is that all the operations pertaining to the preparation, purification, and fabrication of pure materials are performed by Ames Laboratory personnel. Quantities of the ultrapure rare-earth and refractory metals and alloys in single and polycrystalline forms are available providing: (1) the material/service cannot be obtained from a commercial source and (2) that material will not be resold. Students and researchers are welcome to visit the center to learn specific operations on a prearranged basis.

12. For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?

Answer: (B/A in thousands)

	FY 1982 (beginning of MPC)	FY 1983	FY 1984	FY 1985
Reimbursable Research	$150	$205	$210	$250

(Outside of House Laboratory Sales)

13. What is the mechanism by which specific research proposals for experiments at the facility are considered?

Answer: All requests for materials and/or services performed by the MPC must be submitted by the Director of the MPC (515-294-5236 or FTS: 865-5236). The MPC Director's recommendation is reviewed and approved by the Ames Laboratory Director for all purchases in excess of $30,000.

14. How many research proposals have been submitted over the past five years, and how many of these have been approved?

Answer: The purpose of the MPC is the preparation, purification, and fabrication of unique materials that researchers throughout the world are unable to obtain from commercial suppliers. Since the beginning of the MPC, there have been over 375 in-house requests and over 260 out-of-house requests for materials and/or services.

15. How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?

Answer: There have been 440 users from university faculty, staff, and students of the MPC since its beginning in FY 1982.

16. How many industrial researchers have utilized the facility over the past five years?

Answer: There have been 79 requests for MPC materials and/or services from industrial researchers since its beginning in FY 1982.

17. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer: There have been 42 requests for MPC materials and/or services from researchers from foreign institutions since its beginning in FY FY 1982.

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: Fifty-eight researchers from other agencies have used the MPC since its beginning in FY 1982. These have been from NSF, DOD (Army, Navy), NASA, and NBS. Of these 58 researchers, 50% of them are located at universities.

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: Since the beginning of the MPC, we have supplied many researchers with quantities of unique materials which they have used in their various research programs. We expect a gradual increase in these requests over the next several years. In addition, we have been supplying kilogram quantities of the terfenol alloy to five companies interested in developing this magnetostrictive material into prototype sonar devices or into micropositioner devices. In the near term, we intend to help these companies as much as possible develop this technology and to help bridge the gap between what industry can supply and what various government agencies such as DOD need to improve their capabilities.

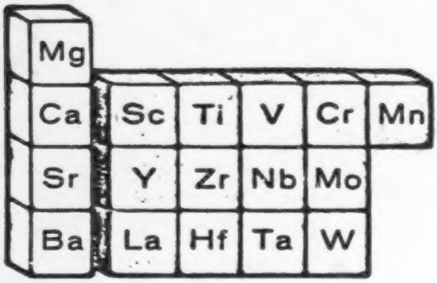
During the course of our basic research sponsored by the Department of Energy, Materials Sciences Program, unique capabilities for preparation, purification, and fabrication of certain metals and materials have in the past been developed. This trend we believe will continue and as a result, materials from these efforts will be available through the MPC to other researchers.

20. Please provide a copy of the facility's latest annual report.

Answer: A copy of the brochure, "Materials Preparation Center" is attached.

Materials Preparation Center

AMES LABORATORY IOWA STATE UNIVERSITY AMES, IOWA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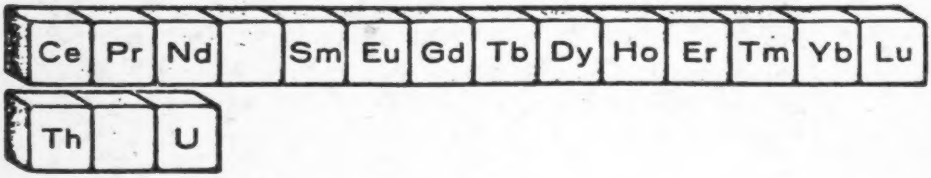
- ● PREPARATION
- ● PURIFICATION
- ● FABRICATION
- ● SINGLE CRYSTAL


Ce
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The Cover: Scanning Electron Micrograph (SEM) of zone-melted Y-5.8 at% Nb showing rod-eutectic structure. Deep-etched with 40% $C_2H_4OHCOOH$, 10% H_3PO_4, 20% CH_3COOH and 30% HNO_3. 3800X

AMES LABORATORY

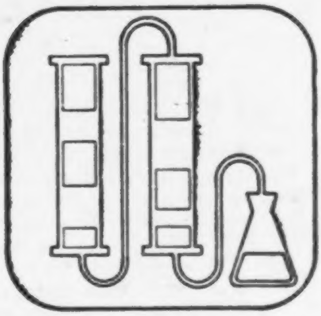
Materials Preparation Center

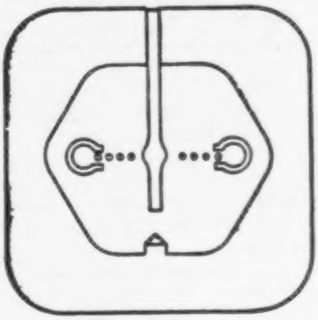
Unique capabilities for preparation, purificati and fabrication of certain metals and materi have been developed by investigators at the Ames Laboratory during the course of their basic research sponsored by the Departmen Energy, Materials Sciences Program. Individ within the Laboratory's Metallurgy and Ceram Program are widely recognized for their worl with very pure rare-earth, alkaline-earth and refractory metals. Similarly, the high-purity metals and alloys prepared at Ames are use extensively by other researchers throughout world. These and other factors have provide impetus for establishment of the Materials Preparation Center (MPC).

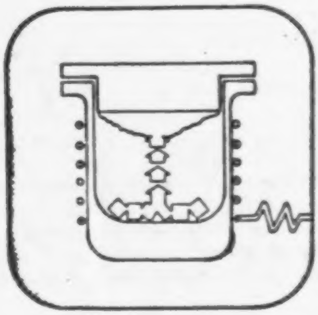
Besides strengthening materials research an development at the Ames Laboratory, the existence of the Center increases awareness the research community of the scope and accessibility of this resource to universities, other government and private laboratories. An attendant benefit of this is the appropriate transfer of unique technologies developed at t Center to private, commercial organizations; a number of such technology transfers have already obtained.

Through these research efforts at Ames, scientists are now able to acquire very high-purity metals and alloys in single and polycrystalline forms, as well as the sophisticated technology necessary to satisfy many needs for special preparations of rare-earth, alkaline-earth, refractory and some actinide metals. The materials are not availabl from commercial suppliers, and through its activities the Center helps assure the research community access to materials of the highest possible quality for their research programs.

Rare-Earth Metals and Compounds





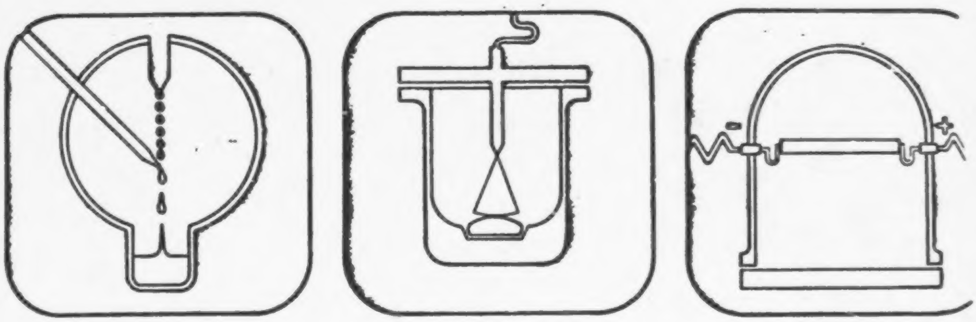


The Ames Laboratory has been actively involved in the preparation of very pure rare-earth metals since the early 1940's, when Dr. Frank H. Spedding and his group of pioneers developed the ion-exchange process, a technique that separates the "fraternal fifteen" plus yttrium and scandium. As a result of this and subsequent work, oxides are available from which rare-earth metals can be prepared. In most cases, the rare-earth oxides are first converted to their respective fluorides and are subsequently reduced metallothermically, on a kilogram scale, using pure calcium metal specially sublimed for this purpose. The resulting metals are very pure. Nonetheless, many are further refined by one of the processes:

- sublimation
- distillation
- vacuum casting
- zone refining
- electrotransport processing

Quantities of ultrapure rare-earth metals and alloys in single and polycrystalline forms are available to scientists outside Ames Laboratory. Complete chemical analyses, obtained by spark-source mass spectrometry, vacuum fusion and combustion analysis, accompany the materials. Special preparations of high-purity oxides and compounds are also available in limited quantities.

Refractory and Alkaline-Earth Metals



As a result of early interest by the Atomic Energy Commission, the Ames Laboratory has engaged in continuing research on the preparation, purification and property determination of refractory metals. Concomitant with successful development of processes for production of uranium and thorium, reduction and casting facilities were put in place in the early 1950's, and have been continuously updated to now include:

- low-pressure, induction casting
- consumable and non-consumable arc-casting
- small-scale, drop casting
- electroslag melting
- electron beam melting

These are among the operations used to develop metallurgical processes for preparing the refractory metals zirconium, hafnium, niobium, molybdenum, tantalum and vanadium. Furthermore, Ames Laboratory has developed and used unique technologies to prepare refractory metals in single and polycrystalline forms, including selective deoxidation and denitrification of the Group V and VI metals, and purification of all the refractory metals in rod, wire and ribbon form by electrotransport processing under ultralow-pressure conditions. Very high-purity, single-crystal rods have been prepared by electrotransport processing specimens purified initially by electron beam, zone refining. All of these materials and forms are available to the research community.

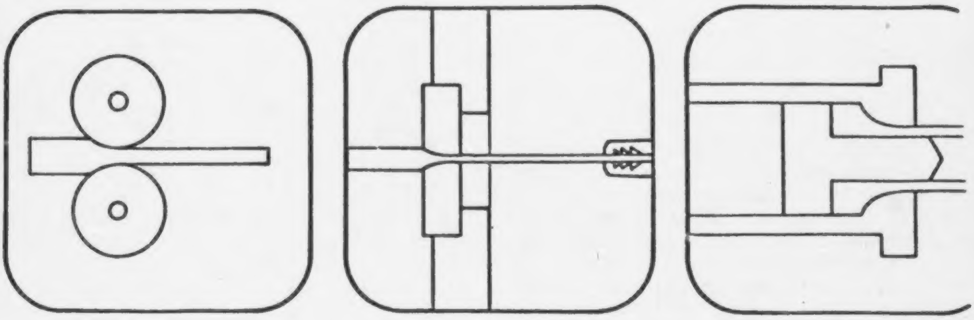
During development of reduction processes for refractory metals, it was necessary to improve the quality of certain alkaline-earth metals used as reducing agents. As a result, high-purity calcium and magnesium have become available, along with high-purity barium and strontium. These metals require special processing to minimize surface contamination prior to use.

Fabrication

Fabrication of high-purity metals and alloys into shapes requisite for specific research studies often requires innovative quality control procedures in order to ensure that specimens are not contaminated during processing. Experience, and the capabilities embodied in the metallographic laboratory and analytical chemistry facilities ensure that the high standards required by Ames Laboratory are met.

The following fabrication operations are routinely performed within the MPC:

- rolling to plate and thin foils
- rod rolling
- swaging
- conventional extrusion
- compacting
- drawing to wire and tubing
- heat treating
- annealing



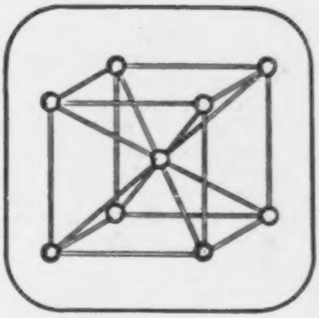
Single Crystals

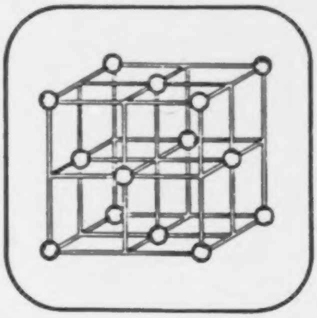
Ames Laboratory is a leader in the preparation of high-quality, single-crystals of rare-earth and refractory metals and their alloys. For 30 years various scientists throughout the world have used these crystals to determine the physical properties of many pure metals and alloys.

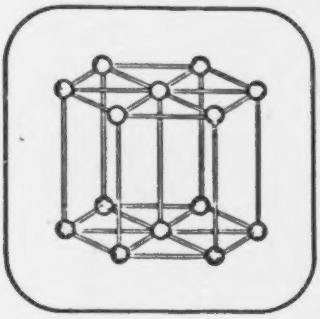
The following techniques are used for preparation of single-crystals in the MPC:

- arc-zone melting
- horizontal, levitation-zone melting
- cyclic-temperature technique
- float-zone melting
- recrystallization-grain growth

High-purity, single-crystals of rare-earth and refractory metals are available, and some crystals can be refined to extreme purity by several metal-purification procedures, such as electrotransport and selective deoxidation. This tandem processing makes available for scientific research metal crystals that are among the purest in the world.







It is not possible to list simply the costs and availability of all the materials and processes in the MPC. These vary from time to time and according to specific requirements. For more information about the Materials Preparation Center and how to obtain materials please contact:

Frederick A. Schmidt
Operations Manager
Materials Preparation Center
121 Metals Development Building
Ames Laboratory
Ames, IA 50011

Telephone: 515/294-5236
FTS 865-5236

2.0 Argonne National Laboratory

2.1 Atomic Spectroscopy Facility

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

   Answer: At this facility scientists are measuring the dynamical properties of polyatomic systems excited into the vacuum-ultraviolet spectral region with spectral and temporal resolution which are unprecedented. These important new measurements will form the basis for the development of a complete description on the microscopic level, of the photochemistry, radiation chemistry, and chemical reactivity of simple molecules.

   These measurements must be done with a temporal resolution that is comparable to the lifetime of the most rapid process, i.e., with picosecond time resolution. For this reason we are continuing our development of the four-wave mixing technique in mercury by extending the technique to produce picosecond duration pulses of vacuum-ultraviolet light. When this source is developed it should provide a factor of seventy (70) improvement in temporal resolution over existing synchrotron light sources and should help us take very detailed and fast pictures of chemical processes and reactions.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

   Answer: One of the principal instruments in this facility, a 30-foot spectrograph which is the only high-resolution instrument in existence in the western world with a complete photographic circle. By filling the entire circle with photographic plates, it is possible to record the entire spectrum of a sample from 210 to 1000 nm at one time. When only a few micrograms of a material are available, this capability is invaluable.

   The uniqueness of a second instrument, the vacuum ultraviolet coherent source (based on four-wave mixing in atomic mercury) lies in the fact that it is the most efficient generator of photons in the 25-220 nm range currently in existence. A similar instrument is under construction for use in the magnetic confinement fusion program by one of the co-developers of this source.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

   Answer:

INSTRUMENT	SPECTRAL REGION (nm)	RESOLVING POWER E/ΔE
30-foot Paschen-Runge spectrograph	200-900	5 x 10(5)
5-meter Czerny-Turner spectrograph	120-500	10(6)
Vacuum-ultraviolet coherent source	110-125	10(7)

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer: An intense source of tunable highly-monochromatic coherent photons in the vacuum-ultraviolet spectral region, in particular, near the important Lymann-alpha line of atomic hydrogen, was developed at this facility. The non-linear technique of four-wave mixing in atomic mercury is used to generate the vacuum-ultraviolet light. The peak spectral flux, i.e., number-of-photons/unit-energy/unit-time, of this source is several orders of magnitude greater than other sources such as: four-wave mixing in rare gases, synchrotron sources with wigglers or undulators, laser generated plasmas, condensed gas sparks, or rare gas continua. The source is now being used for basic research in atomic, molecular, and chemical physics and its use to monitor the temperature and spatial properties of Tokamak fusion devices is planned.

Absolute photometric measurements are not possible with photographic plates, but they are possible with diode-array detectors. Such a detector has been installed on our five-meter vacuum-ultraviolet spectrograph. With this detector we have measured the line shape and absolute intensity of transients in atomic barium as a function of barium number density. The results of these measurements were used to identify collision-induced transitions in atomic barium. At a barium number density of approximately 10^{20} atoms-m^{-3} collision-induced transitions were identified. These transitions are induced by the electric field which is produced by the ions and results from the finite autoionization probability. At the relatively low ion number densities of 10^{15} to 10^{16} ions-m^{-3}, which represents between 0.01% and 0.001% of the neutral barium atoms converted to ions, the induced transitions are easily observed. These observations show the sensitivity and precision with which diode arrays may be used to make photometric measurements.

The discovery of the quasi-Landau resonances in atomic barium and strontium pointed out the importance of coupled electronic motion when the Coulomb field produced by the nuclear charge and core electrons of an atom is of the same order of magnitude as an externally applied magnetic field. Also, the importance of doubly-excited states, i.e., states where the excitation energy is shared between two electrons as opposed to single-electron states where all the excitation energy resides in a single electron, was established at this facility. Recent measurements of the transition rate for two-photon resonant, three-photon ionization transitions, which were made in the spectral region where doubly-excited and single-electron-excited states interact, have shown that the line profiles of the resonant transitions are very sensitive to the polarization and intensity of the exciting light. These results are currently being used to reassign certain transitions and to formulate a more complete theoretical description of the multi-photon transition process.

It is anticipated that the techniques developed to produce highly-monochromatic coherent photons will be extended to provide intense picosecond duration pulses of light in the vacuum-ultraviolet spectral region. Such a source does not exist at the present time, therefore, when developed, it should provide about a factor of seventy (70) improvement over the time resolution of existing synchrotron light sources. This improvement, when used in conjunction with the already existing high spectral flux of the source, i.e., photons/unit-energy/unit-time, will allow scientists to excite specific states of polyatomic systems and monitor the evolution of the system with a time resolution comparable to the characteristic time of the fundamental molecular processes.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: A five-meter vacuum-ultraviolet spectrograph was obtained from a DOD laboratory and brought to this facility. The spectrograph was installed, refitted with an efficient holographic grating, and modified to use both photographic and diode-array detectors. Experimentation with this instrument began in FY 1983.

A vacuum-ultraviolet coherent source, developed through research on four-wave mixing in atomic mercury, was added to the facility in FY 1983. It is anticipated that the four-wave mixing process in mercury will be extended to produce pico-second duration pulses of light in the vacuum-ultraviolet spectral region. This development should be complete in FY 1984 with experiments beginning in FY 1985.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer:

Budget Profile

Budget Authority in Thousands

	FY81	FY82	FY83	FY84	FY85	Source of Funds
Operating Costs	69	80	87	87	64	Chemical Sciences
In-House Research	313	362	394	388	290	Chemical Sciences
Out-of-House Research	20	20	20	20	20	Chemical Sciences
Capital Equipment	16	42	38	45	70	Chemical Sciences

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer: None.

8. **For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.**

Answer:

	FY81	FY82	FY83	FY84	FY85
Man-years (Operations)	1.0	1.0	1.0	1.0	0.5
Man-years (Research)	2.0	2.0	2.1	1.8	1.4
Total	3.0	3.0	3.1	2.8	1.9

9. What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?

Answer:

INSTRUMENT	FY81	FY82	FY83	FY84	FY85
30-foot UV-VIS spectrograph	0.25	0.25	0.50	0.25	0.25
5-meter VUV spectrograph	0	0	0.50	0.50	0.50
VUV coherent light source	0	0	0.50	1.00	1.00

The above values represent fractional utilization, i.e., 1.00 is full utilization. Full utilization represents use 8 hours per day, 5 days per week.

10. For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?

Answer:

Number of experiments (FY81-FY85):

Number of experiments started	101
Number of experiments continued	20
Number of experiments completed	81

11. What is this facility's user policy?

Answer: This facility, while not an official user facility, is open to all qualified users. Experiments by outside users are encouraged. Potential users arrange an experimental schedule which is appropriate for both the user and the in-house scientists. The majority of such experiments are collaborations with in-house scientists.

12. For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?

Answer: None.

13. What is the mechanism by which specific research proposals for experiments at the facility are considered?

Answer: As noted in the answer to Question 11, this is not officially a user facility. The small number of visitors, all highly qualified, almost invariably do so in collaboration with ANL scientists. There have been fewer than 4 such visitors per year, each visit occupying 2 weeks or so.

14. How many research proposals have been submitted over the past five years, and how many of these have been approved?

Answer: Approximately ten experiments have been arranged with researchers other than DOE or contractor personnel. All requests to use the facilities have been approved.

15. How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?

Answer: Fifteen (15) university personnel have utilized the facility in the past five years.

16. How many industrial researchers have utilized the facility over the past five years?

Answer: Two (2) industrial researchers have utilized the facility in the past five years.

17. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer: Seven (7) researchers from foreign institutions have utilized the facility in the past five years.

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: None. ("Researchers from other agencies" are defined as regular employees of agencies, federal or state, other than DOE or GOCO contractors.) It should be noted that scientists from other DOE laboratories use this facility.

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: There are many potential future development possibilities for the existing Atomic Spectroscopy Facility, but there are currently no specific plans to undertake any of them beyond the construction activities identified in the FY 1985 budget request.

20. Please provide a copy of the facility's latest annual report.

Answer: No formal reports on facility use are prepared, since this is not operated as a formal user facility. Reports of research accomplishments, which include the work of outside collaborators and users, are prepared for DOE - Chemical Sciences in the Field Task Proposals and in an annual report, "Surveys of Research in the Chemistry Division" prepared for our Review Committees and general interest. A copy of the relevant pages from the most recent "Surveys of Research in the Chemistry Division" is included.

VI. HIGH-RESOLUTION SPECTROSCOPY AND EXCITED-STATE DYNAMIC PROCESSES

(H. M. Crosswhite, F. S. Tomkins, K. T. Lu, B. Ercoli, J. F. Kelly)
Outside Collaborators (H. Crosswhite, P. M. Dehmer, W. R. S. Garton, J. F. Kielkopf, M. H. Nayfeh, W. H. Parkinson, P. L. Smith)

High-resolution spectroscopy has a long and distinguished history at ANL. While earlier efforts were directed toward unraveling the energy level structure of the actinide elements, recent emphasis has shifted to the study of Rydberg states in applied magnetic fields, and to the generation of vacuum-ultraviolet radiation *via* non-linear mixing in atomic vapors. This basic research program is in a transition phase. The combined experimental and theoretical program, which emphasized energy level measurements and calculations, is being replaced by an experimental program which will study spectroscopic properties and dynamic processes of highly-excited atomic and molecular systems. This shift in emphasis is due to the unique capabilities, developed at ANL, for the generation of intense, pulsed, narrow-band, and tunable radiation in the vacuum-ultraviolet region (5 to 10 eV). This program, which is based upon laser techniques, will also be reinforced by the more conventional dispersive spectroscopic techniques for initial spectral studies and for complementary studies of selected spectral regions. The unique ANL facilities for these high-resolution applications now also include a choice between photographic or photoelectric detection by means of computer-controlled diode-array detectors. The vacuum-ultraviolet spectral region is particularly interesting because molecular processes, such as reactive ionization, reactive dissociation, and the interaction between channels, may only be studied at excitation energies in excess of 5 eV. Initial experiments include studies of the line profile of the Lyman-α transition (1s-2p) in atomic hydrogen and excitation and fluorescence lifetime measurements of the D $^2\Sigma^-$ state of the hydroxyl radical, OH. The criteria for selecting chemical systems for study are (1) their appropriateness to test theoretical concepts, and (2) their fundamental bearing on chemical and energy technologies.

A. Rydberg States of Two-electron Systems (H. M. Crosswhite, F. S. Tomkins, B. Ercoli, H. Crosswhite, W. R. S. Garton, J. F. Kelly, J. F. Kielkopf, M. H. Nayfeh)

(1) Absorption Line-Profile Measurements of Transitions in an Applied Magnetic Field

In 1969, Garton and Tomkins discovered a dramatic modulation, now known as the quasi-Landau resonances, in the absorption spectrum of barium in a magnetic field of 2.5 Tesla. Later, Fonck *et al*. observed diamagnetically-induced configuration mixing in laser-excited barium. In this work, line profiles for strontium and barium were found to differ significantly. This new class of phenomena has generated a great deal of interest and challenge because the applied fields and the diminished Coulomb field experienced by an electron in a highly excited Rydberg state are comparable. Also, in two-electron systems (*e.g*. the alkaline-earth atoms Ba and Sr) the Rydberg and doubly-excited states are coupled differently to the magnetic field.

In the past, a great deal of effort has been devoted to the analysis of measurements of the energy intervals between Rydberg states. Interest in oscillator strengths, line profiles, and collisional processes has been barely pursued. In addition, previous work has been confined to the wavelength region longer than 200 nm. There is a pressing need to extend all types of measurements to the shorter wavelength, vacuum-ultraviolet region. To perform such studies, we have set up a diode-array detector on our 5-meter vacuum-ultraviolet spectrograph. Because quantitative absorption measurements can now be performed and analyzed on the time scale of seconds to minutes, detailed measurements of both the energy interval and, of greater importance, the oscillator strength and line profile may be performed in the critical regions of applied magnetic field where states strongly interact. Measurements are underway on the absorption line profiles near the ionization limit of barium. These results will provide the first quantitative measurements as a function of magnetic field. Such measurements will yield very precise and detailed information on the magnetically-induced interaction between coupled configurations, and, as such, will provide a more detailed assessment of current theoretical concepts and calculations.

(2) Absolute Cross Section Measurements of Radiative Transitions to Mixed Levels

Even in the absence of an applied magnetic field, the Rydberg and doubly-excited levels of the alkaline earths strongly interact. This interaction has recently been studied in a number of laboratories: at JILA, by measurements of the angular distribution of photoelectrons following resonant multiphoton ionization; at the Freie Universität Berlin, by measurement of the hyperfine-induced mixing in ^{87}Sr; and, at the Laboratoire Aimé Cotton, by lifetime measurements of the 6snd $^{1,3}D_2$ Rydberg levels of Ba. The analysis of any measurement of the lifetime of a Rydberg level involves the summation over many transition probabilities. Our approach is to measure the absolute absorption cross section of transitions to mixed levels, thereby isolating a single transition probability. Because the measurement of an absorption cross section probes the wavefunctions of only the initial and final levels, these measurements will provide a more sensitive probe of wavefunction mixing. Systematic studies of the amount of wavefunction admixture will be performed by measuring the cross sections as a function of the effective principal quantum number of the Rydberg level.

Measurements of the two-photon absorption cross sections for transitions from the $6s^2\ ^1S_0$ ground level to the 6snd $^1D_2$ Rydberg levels of barium are in progress. Near $n = 27$, the Rydberg levels strongly interact with the doubly-excited 5d7d $^1D_2$ level. These cross sections are measured by carefully monitoring the two-photon excitation intensity, saturating the single-photon, 6snd $^1D_2$-to-continuum transition, and detecting the Ba ion yield. In addition to providing information on the interaction between configurations, this work is also establishing fundamental techniques for the measurement of two-photon absorption cross sections.

B. Dynamical Processes of Excited States (F. S. Tomkins, P. M. Dehmer, J. F. Kielkopf, W. H. Parkinson, P. L. Smith)

(1) Collisional Properties of Atomic and Molecular Hydrogen

The interpretation of spectroscopic measurements of collisional processes involving alkali atoms and dimers has been hampered by the complex electronic structure of the system. Analogous studies of atomic and molecular hydrogen offer opportunities for precise interpretation of experimental results. In addition, because of the low mass and near degeneracy of the electronic states of atomic hydrogen, effects which are masked in other systems may be observed in atomic hydrogen. Until now, experimental techniques for the study of collisions involving H or H_2 have been limited to classical spectroscopic techniques. With our recently developed vacuum-ultraviolet source, we are in a position to perform unique measurements of the collisional properties of atomic and molecular hydrogen. Recent experiments have shown that resonant excitation and fluorescence experiments on atomic hydrogen can be performed under the conditions necessary for the study of collision processes.

(2) Properties of the D $^2\Sigma^-$ State of the Hydroxyl Radical

The hydroxyl radical, OH, is an important constituent of interstellar clouds, the comae of comets, the earth's upper atmosphere, ambient air (even though it is highly reactive), and any combustion process involving hydrogen. For example, the reaction of OH with ozone is important to the formation of smog in urban areas. Also, laser-excitation of the OH radical has been postulated to be an effective technique for modifying combustion processes.

All spectral diagnostic and excitation techniques have employed the A $^2\Sigma^+$ state of OH. Of its five known bound states, the D $^2\Sigma^-$ state is also a potentially useful diagnostic state. In addition, because D ← X absorption leads to dissociation of the radical, the dynamic properties of the D state are of fundamental interest to astrophysicists. The absorption cross sections for D ← X transitions and the radiative decay rates of the vibrational levels of the D state have recently been calculated to be much stronger than the analogous properties of the A state. Therefore, the D state may prove to be of greater utility and/or sensitivity, both for spectral diagnostics and for modification of combustion processes, than the the well-studied A state.

We are now employing our recently developed, non-linear mixing technique to perform laser-excitation and fluorescence lifetime measurements of the D $^2\Sigma^-$ state of OH. The excitation measurements include a search for the $v' = 1$ vibration level of the D state, which, if observed, would provide an assessment of the recent theoretical calculation of the potential energy curve of this state. The lifetime measurements are the first studies of the dynamic properties of this potentially important state.

2.2 4.5-MV Dynamitron Accelerator

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

   Answer: The new science pursued at this facility is to understand the structure and the motion of atoms and of molecules that are deficient in electrons. These entities are called ions; in one case they may be charged single atoms and in the other case, one aggregate of atoms that is charged. Since the electrons themselves are negatively charged, their removal from an atom or a molecule leaves a positively charged particle. One paramount importance of this result is that they can then be manipulated with electric and magnetic fields. This property permits control of their energy and motion that is necessary to determine their character. The study of their structure and motion is enhanced by noting under what conditions and circumstances their ions emit light. By examining the nature of this light, its intensity and its energy, the physics required can be extracted. The measures of all these characteristics are made at the Dynamitron facility with the best possible precision in order to discard any artifact that appears in the data and to allow for a stringent test of theory that attempts to explain these phenomena and to predict new ones. The use of lasers in this laboratory enhances our ability to follow the motion of these ions with the highest precision currently possible. The ions themselves can be made to move faster or slower by changing the size of the magnetic and electric fields that are used to control their motion. Thus very fine manipulation of the interaction between laser light and ions is possible.

   The results are important because they tell us in the most fundamental manner possible how light interacts with matter at the atomic level. Since all matter is made up of atoms, we can begin to understand how charged aggregates of atoms are located in space relative to one another at a level of precision previously not possible. These experiments also make it possible to understand precisely how energy can be transferred from one atom to another such as when an ion strikes a surface, as happens in a fusion plasma, or in etching a circuit to produce a computer chip.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

   Answer: The accelerator is unique because of the combination of the intense beam current, exceptionally high angular resolution and a wide range of sophisticated technical support apparatus, including a beam line capable of providing "supercollimated" ion beams permitting angular measurement to accuracies of 0.005 degree, an experimental system dedicated to measuring absolute nuclear cross sections at low energy, a laser-ion beam-interaction beam line where laser beams from an argon pump and a dye laser are available coaxially and simultaneously with the Dynamitron ion beam, and a post-acceleration chopper system giving beam pulses of variable width from about one nanosecond to the millisecond range at repetition rates variable up to 8 MHz.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

Answer: Among the facilities associated with the Physics Division's 4.5-MV Dynamitron accelerator are (1) a beam line capable of providing "supercollimated" ion beams permitting angular measurement to accuracies of 0.005 degree, (2) a beam-foil measurement system capable of measuring lifetimes down to a few tenths of a nanosecond, (3) an experimental system dedicated to measuring absolute nuclear cross sections at low energy, (4) a variety of experimental apparatuses for weak-interaction studies, (5) a laser-ion beam-interaction beam line where laser beams from an argon pump and a dye laser are available coaxially and simultaneously with the Dynamitron ion beam, (6) a post-acceleration chopper system giving beam pulses of variable width from about one nanosecond to the millisecond range at repetition rates variable up to 8 MHz, (7) a scattering chamber for electron spectroscopy incorporating electrostatic parallel-plate electron spectrometers with variable energy resolution (0.1% to 5%) and the capability to measure electron energies up to a few keV as a function of observation angle, and (8) two general-purpose beam lines used for a variety of short-term experiments. A PDP-11/45 computer system is used for on-line data analysis and for the control of experiments.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer: Some of the major research highlights for the period FY1981-85 include:

a) The first precise measurement of the process by which two atoms initially bound together to form a singly charged particle come apart as they travel through a thin gold crystal.

b) The first experiment on how the charged molecule (molecular ion) of hydrogen gas comes apart when ultraviolet light from a laser strikes the molecular ion.

c) The first confirmation of the structure of two simple molecular ions and thereby establishing a brand new technique to study geometric structures of molecular ions.

d) The discovery of the manner by which the electrons immediately separated from atoms can travel together next to the parent ion and yet be independent from it.

e) The first observations of how ions that go through foils of carbon can exit in a form that has only been seen previously when the same species are in the presence of an electric field.

f) The time sequenced determination of the process by which a molecular ion comes apart after it has been made to enter a thin foil and emerges from it in fragments.

g) Highly precise measurement of the time it takes an atom to emit light after it is first perturbed into a condition to do so; measures that provide an account of the environment in which such atoms find themselves, such as observing the behavior of an atom in a fusion plasma.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: The upgrading of the Dynamitron accelerator from a maximum voltage of 4 MV to 5 MV is the primary change occurring at the facility. Already completed are the rebuilding of the toroidal high-voltage transformer and the installation of a new accelerator column structure. Among the modifications in progress are the installations of: 1) a new accelerator tube, 2) a high-pressure insulating gas-handling system, 3) new high-voltage rectifiers, 4) a new computer system for Dynamitron operations. Further improvements include the addition of mass analysis and terminal pumping to the ion sources to reduce loading of the accelerator tube thereby allowing higher operating voltages. New ion sources will be developed to obtain new ion species. Changes in the experimental area include a new beam line with appropriate vacuum pumping to study laser/ion-beam interactions. Two beam lines are now used for general purpose work and for a variety of short-term experiments. Several quadrupole-focussing magnets and one additional bending magnet have been installed on several beam lines for improved ion-beam quality.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer:

(Budget Authority in Thousands)

	FY81	FY82	FY83	FY84	FY85
Operations					
In-house research	439	413	372	411	440
Materials science	108	53	0	0	0
Chemical sciences	248	252	279	308	374
Low-energy nuclear physics	83	108	93	103	66
Out-of-house research	0	0	0	0	0
Other	0	0	0	0	0
Capital equipment	10	0	39	45	50
Other construction (AIP)	0	0	300	100	150

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer: There is no funding from other federal agencies, state agencies, foreign institutions, or private sources.

8. **For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.**

Answer: Staffing Levels for Dynamitron

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operations (FTE)	6.2	5.2	4.6	4.6	4.6
In-house Research (FTE)	8.0	8.0	8.0	8.0	8.0
Total (FTE)	14.2	13.2	12.6	12.6	12.6

9. What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?

Answer: Facility Utilization (Hours)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Staffed time	5344	5380	3808	3800	3800
Scheduled time	3960	4729	3021	3000	3400
Down time	1384	651	787	800	400
Beam available	3109	4257	2759	2700	3000
Preparation time	280	295	191	200	300

Full utilization, i.e., use of the facility for the conduct of experiments, is defined as funded (staffed time) less time scheduled for maintenance or improvements (down time). Theoretical full utilization of this facility would be about 7200 hours per year.

10. For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?

Answer: Because of the nature of the research performed with the Dynamitron, it is difficult to define the "start" and "end" to experiments. We instead tabulate the number of requests for beam time and the number of publications concerning work at the facility each year. (Note that several "beam time requests" may comprise one experiment.)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Requests	46	60	37	50*	50*
Publications	26	22	19	N/A	N/A

* Extrapolated based on 1st quarter of FY 84.

11. What is this facility's user policy?

Answer: The Dynamitron is not an official user facility; however, we accommodate outside users and we encourage the active collaboration of outside users in our in-house research programs. Projects suggested by outside users should be relevant to these programs and the results must be published in the open literature.

12. For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?

Answer: None.

13. **What is the mechanism by which specific research proposals for experiments at the facility are considered?**

Answer: None exists since the Dynamitron Accelerator Laboratory is not an official "User" facility.

14. **How many research proposals have been submitted over the past five years, and how many of these have been approved?**

Answer: Not applicable.

15. **How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?**

Answer: There have been 71 outside university users of the facility during the past 5 years.

16. **How many industrial researchers have utilized the facility over the past five years?**

Answer: There were no industrial researchers utilizing the facility over the past 5 years.

17. **How many researchers from foreign institutions have utilized the facility over the past five years?**

Answer: There were 10 researchers from foreign institutions using the facility during the past 5 years.

18. **How many researchers from other agencies have utilized the facility over the past five years?**

Answer: There were 3 researchers from other agencies that have utilized the facility over the past five years. ("Researchers from other agencies" are defined as regular full-time employees of agencies, federal or state, other than DOE or GOCO contractors.) It should be noted that scientists from other DOE laboratories use this facility.

19. **What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?**

Answer: The Dynamitron continues to be a unique facility for obtaining high-current ion beams with high energy resolution. These features can be enhanced further. Future development possibilities also include expansion of our program of determining stereochemical structures of molecular ions. As this program proceeds, it is foreseen that the ion source capabilities will be extended to include new species of molecular ions, including negative ions. The budget will not be significantly affected.

20. **Please provide a copy of the facility's latest annual report.**

Answer: There is no annual document prepared addressing solely the Dynamitron and its application. However, each year the Argonne Physics Division issues a summary of research activities entitled "Physics Division Annual Review." The relevant pages from "Physics Division Annual Review, 1 April 1982 - 31 March 1983" are enclosed.

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ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

PHYSICS DIVISION ANNUAL REVIEW
1 APRIL 1982—31 MARCH 1983

Donald S. Gemmell
Division Director

June 1983

Preceding Annual Reviews

ANL-80-94	1979—1980
ANL-81-79	1980—1981
ANL-82-74	1981—1982

We are presently studying the beta decay of polarized ^{8}Li, produced with a polarized deuteron beam on a cold target of ^{7}Li metal kept in a magnetic holding field. The asymmetry between up and down polarization states is detected by two electron-detection telescopes. Total electron energy is measured in large plastic scintillators. This investigation will therefore yield the energy dependence of the decay asymmetry. Data from our first run are being evaluated and the detector is being refined.

c. A Test of V-A Positron Decay (S. J. Freedman, G. T. Garvey, J. Napolitano and A. Rich*)

We are considering a possible experiment to measure the helicity of positrons from nuclear positron decays as a sensitive test for the presence of V + A currents. The experiment would utilize a novel and very sensitive polarimeter for positron helicities developed by A. Rich and co-workers at Michigan. The method utilizes the spin dependence of positronium annihilation in a magnetic field as a measure of the positron spin. A possible experiment would require intense sources of ^{26}Al^m and ^{30}P that could be produced either at the Dynamitron or the Argonne Cyclotron. A feasibility study is currently underway.

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*University of Michigan, Ann Arbor, Michigan.

d. The Beta Decay Rate of ^{16}N($J^\pi = 0^-$, 120 keV); Meson Exchange Currents and the Induced Pseudoscalar Coupling Constant (C. A. Gagliardi, G. T. Garvey, S. J. Freedman, and J. R. Wrobel)

We have improved (by a factor 2) our previous measurement of this important decay. The bulk of the error in the 0^- beta decay rate now rests with the uncertainty in the decay rate of the $J^\pi = 2^-$ ^{16}N ground state which is under investigation. Apart from this error, currently at 11%, we have reduced all other sources of error in this decay branch to 4%. The improvements in the measurement over our earlier result involve higher statistics and more uniform targets.

The $0^- \rightarrow 0^+$ decay rate is important for quantifying the role of pions in the nuclear medium. A pseudoscalar transition such as this one is believed to be effected strongly by the presence of pions in nuclei. Their strong effect on this transition is just a consequence of the time-like component of the axial vector current. Sizable meson exchange effects have long been predicted and detailed calculations have recently been carried out for the $^{16}N\ 0^- \rightarrow 0^+$ case. Thus this particular measurement is significant as it represents a case where the nuclear structure is both simple and calculable and the μ capture rate between the ^{16}O ground state and the $^{16}N, J^{\pi} = 0^-$ 120-keV level is well known ($\Lambda_\mu = 1560 \pm 94\ \text{sec}^{-1}$). This ratio of the μ capture rate to the beta decay rate is very sensitive to the pion currents and insensitive to the details of nuclear structure. Figure I-12 shows the comparison of theory to the measured decay probability (Λ_μ) along with our measured value of the beta decay probability (Λ_β).

The difficulty in measuring the beta decay rate arises from the fact that it is a weak decay of an excited state with an electromagnetic decay rate of $\Lambda_\gamma = 1.32 \pm 0.02 \times 10^5\ \text{sec}^{-1}$. Thus the beta decay branch is the order of 10^{-6} of the total decay probability for this level. Using techniques described in last year's submission we have measured $\Lambda_\beta = 0.45 \pm 0.05\ \text{sec}^{-1}$. Figure I-13 shows the beta rate measured as function of time with respect to a peak burst over an 18-hour run. As stated in the opening paragraph of this section the bulk of the error lies in the ^{16}N ground state to ^{16}O ground state decay branch which is used to calibrate the efficiency of our beta detector system. This work has led to two invited talks and a Physical Review Letter. A more detailed Physical Review article is nearing completion.

e. $0^+ \rightarrow 0^-$ Beta Decay of ^{16}C Ground State (C. A. Gagliardi, G. T. Garvey, N. Jarmie,* and R. G. H. Robertson*)

As part of the effort to establish the role of virtual pions in nuclei we have measured the beta decay of the ^{16}C ground state to the 0^-, 120-keV level of ^{16}N. These pseudoscalar matrix elements are known to be

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*Los Alamos National Laboratory, Los Alamos, New Mexico.

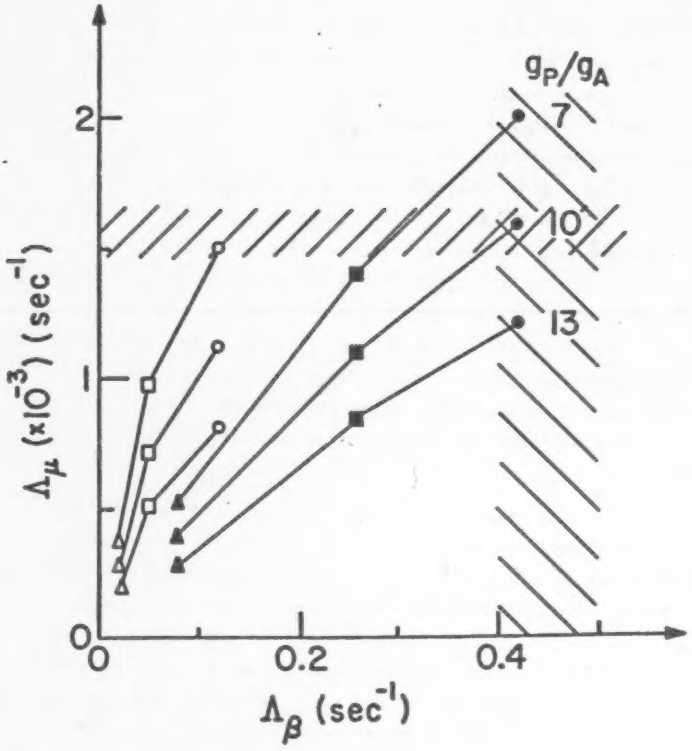

Fig. I-12. Calculation of Towner and Khanna, Nucl. Phys. A372, 331 (1982) compared to experimental value for Λ_μ and Λ_β. The open points are the result of impulse approximation calculations while the closed points include meson-exchange currents. Curves are shown for 3 values of g_P/g_A.

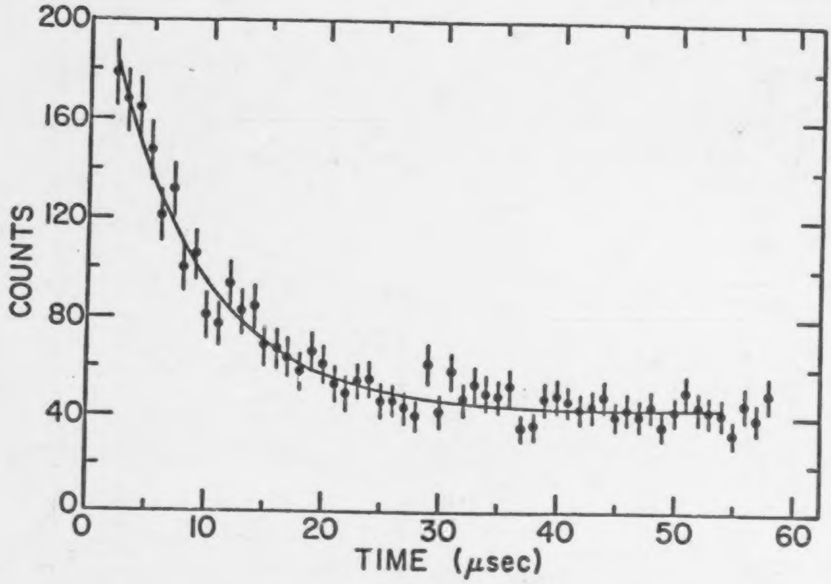

Fig. I-13. The rate as function of time observed in the beta telescope. The smooth curve is a fit to an exponential (τ = 7.8 ± 0.7 μs) plus a constant background.

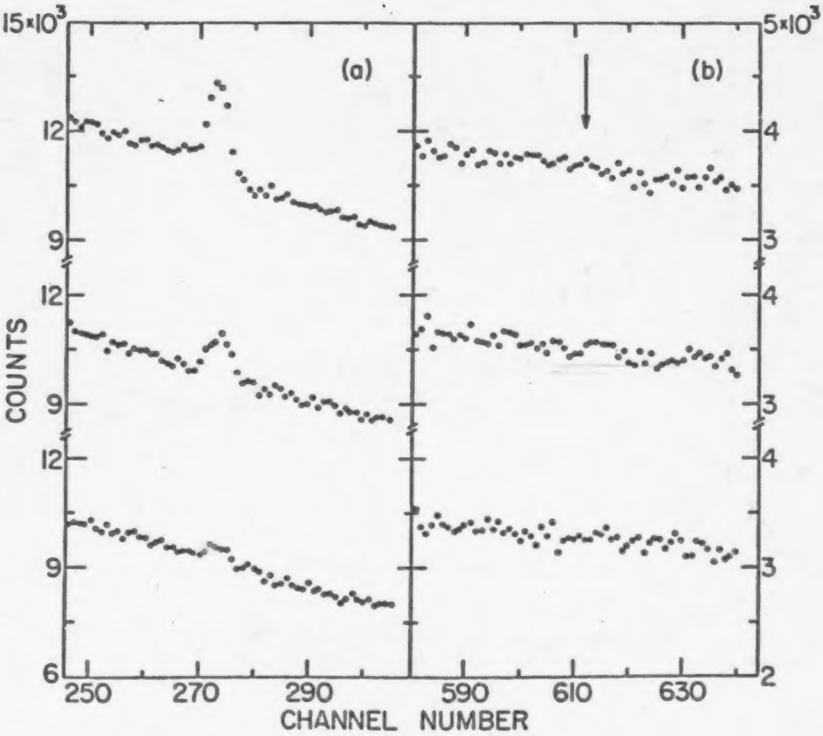

Fig. I-14. The gamma-ray pulse-height spectrum in the region of the 120-keV line for 3 different time intervals. The top spectrum is from the first time bin. The middle spectrum is taken 0.88 sec. later and the bottom spectrum is taken 1.94 sec. later. Note ^{16}O has a 0.75-sec. half life.

greatly affected by pion exchange currents and further the transition matrix elements are very similar to those required to produce $\Delta T = 1$ parity mixing in hadronic systems. This experiment represents the first time that the 0^- branch has been observed in the decay of ^{16}C. The measurement was carried out at the LANL Tandem Van de Graaff, where ^{16}C was produced via the $^{14}C(t,p)^{16}C$ reaction at $E_t = 6.0$ MeV. The use of both a radioactive beam and target allowed the preparation of a much cleaner and stronger ^{16}C source than had heretofore been possible. The prominent decay modes of the ^{16}C ground state are to $J^\pi = 1^+$ neutron unstable states in ^{16}N. We detected the neutrons with a stilbene crystal, the betas in a thin (0.8 mm) plastic scintillator and photons in a 12.5 cm^3 Ge(Li) detector. The absolute efficiency of the Ge(Li) was fixed with calibrated sources while the beta counter efficiency was determined at ANL using $\beta - \gamma$ coincidences in the $^{20}F \rightarrow {}^{20}Ne$ decay. Our results for the ^{16}C decays are a branching ratio of $6.8^{+0.9}_{-1.1} \times 10^{-3}$ for the decay to the 0^- state and a limit of $<10^{-3}$ for the branch to the 1^- state. Figure I-14 shows the γ-ray energy spectrum as a function of time in which the branch to the 0^-, 120-keV line is clear.

As this $0^+ \rightarrow 0^-$ decay depends principally on $2S_{1/2} \rightarrow 1P_{1/2}$ transitions the rate depends on the amount of the $(2S^2_{1/2})$ component in the ^{16}C ground state. Using an estimate of this component by D. Kurath and our earlier value for the $^{16}N(0^-) \rightarrow {}^{16}O$ ground-state decay rate, we predict a value of the $0^+ \rightarrow 0^-$ branch that is 2.5 times what we observed. A proper calculation of the nuclear structure must be done to determine if we have achieved a quantitative characterization of these pseudoscalar transitions.

f. The Branching Ratio to the ^{16}O Ground State for the ^{16}N Ground State (A. Heath and G. T. Garvey)

The branching ratio for ^{16}N ground-state decay to the ^{16}O ground state and 6.13-MeV level are 26 ± 2% and 68 ± 2%, respectively. Unfortunately, the errors in these determinations are highly correlated so that the ratio of these branches is $26 \pm 2/68 \mp 2 = .385 \pm .040$. This uncertainty is responsible for the bulk of the 11.5% error in our recent measurement of the beta decay rate of the ^{16}N $J^\pi = 0^-$, 120-keV level as it entered into the calibration of the beta detector efficiency. Reducing the error in the above ratio to 5% would reduce the error in the 0^- branch to 6.9%.

The measurement of the ^{16}N ground-state decay is being carried out at the Dynamitron using the ^{15}N(d,p)^{16}N reaction at E_d = 1.7 MeV. The beta rays are being measured in our flat-field beta spectrometer. The absolute acceptance of the spectrometer is being measured employing β-γ coincidences in the decay of ^{20}F made via ^{19}F(d,p)^{20}F. We expect to be able to calibrate the absolute efficiency of this spectrometer to 3--4% thereby being able to measure the ^{16}N branching ratio to an acceptable level. This device will also be employed to measure the beta spectra associated with the fission of ^{255}Cf, an experiment which bears on the questions of γ spectra associated with heavy fissioning nuclei (U^{235}).

g. Neutron Beta Decay (S. J. Freedman, D. Dubbers,* Y. Last,* P. Bopp,* H. Schütze,* and O. Schärpf†)

Neutron beta decay represents a unique opportunity to study the semileptonic weak interaction in a tractable hadronic system. The first run of a new-generation neutron beta decay experiment was conducted in 1982 at the Institut Laue-Langevin reactor by a collaboration consisting of scientists from Argonne, Heidelberg, and the ILL. The experimental goals are to provide a new high-precision value for the average reaction asymmetry parameter $\bar{A}$, a test of the conserved vector current hypothesis through a measurement of the energy dependence of A, and a value for the neutron lifetime (at the 1% level) by a new experimental method.

The experimental instrument consists of a ~2m long superconducting solenoidal spectrometer equipped with two scintillation detectors. A novel geometry allows us to observe polarized neutron decay over a large region and thus along with the high flux polarized beam at the ILL, the resulting count rates are more than two orders of magnitude higher than previous experiments. The first run of the experiment was completely successful. Data obtained during the run should provide a value of $\bar{A}$ with

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*Physikalisches Institut, Heidelberg, Germany.

†Institut Laue-Langevin, Grenoble, France.

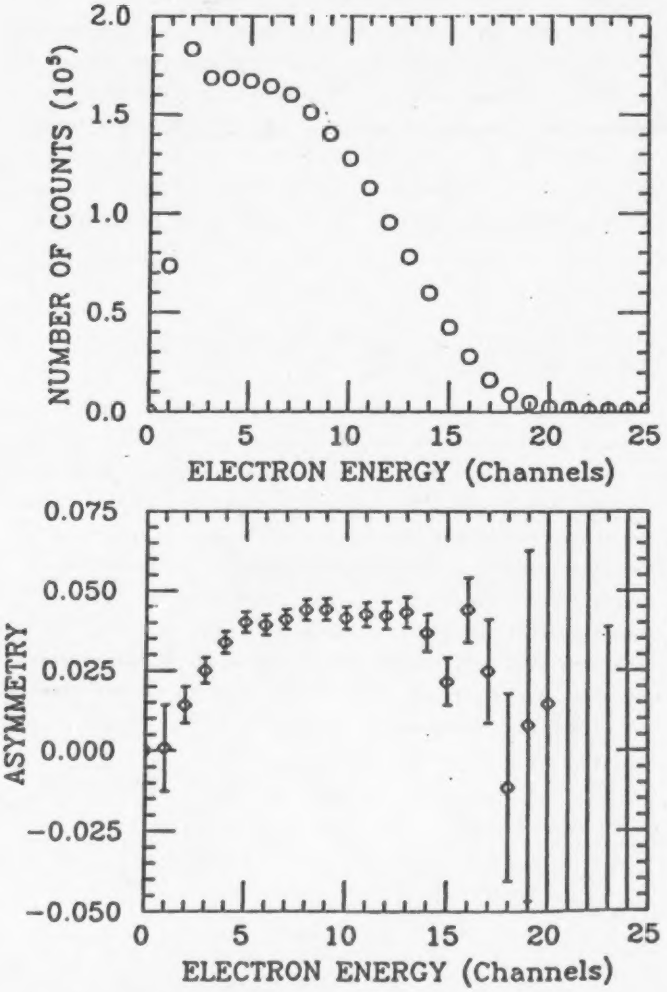

Fig. I-15. Preliminary results on the β-decay asymmetry of the neutron. The upper figure shows a typical background-subtracted electron energy spectrum. Some unsubtracted background remains at this time at low energies. The lower spectrum shows, as a function of electron energy, the asymmetry from polarized neutron β-decay.

an error five times smaller than the best present values. The v/c dependence of the asymmetry was observed for the first time and the data are sufficient for providing a preliminary result for the energy dependence of A. (See Fig. I-15.) The ILL management has allocated three running periods for this experiment during the last half of 1983. The data from the first run are being analyzed at Heidelberg and Argonne and the experiment is being refined and improved for the next run. Application of the present detector to the measurement of other correlation coefficients is under study.

h. Study of the $^{10}B(2^-$, 5.11 MeV) and $^{10}B(2^+$, 5.16 MeV) Levels

(S. J. Freedman and J. Napolitano)

To better evaluate the feasibility of a new effort to study nuclear parity mixing due to the weak neutral current in ^{10}B, we have begun a study of the 2^--2^+ doublet in ^{10}B. The resonance width of the 2^- level has been measured with the $^6Li(\alpha,\gamma)^{10}B$ reaction. (See Fig. I-16.) Values for the total gamma decay width and the gamma decay branching ratios of these levels were also obtained. Future experiments will be performed to measure the α partial-wave decomposition in the $^6Li(\alpha,\gamma)^{10}B$ reaction as well as the branching ratios for particle and gamma decays from the 2^+-2^- doublet. These results will help implement a reevaluation of the current theoretical expectation for parity mixing in ^{10}B. Possible new experiments to measure parity mixing in ^{10}B are being explored.

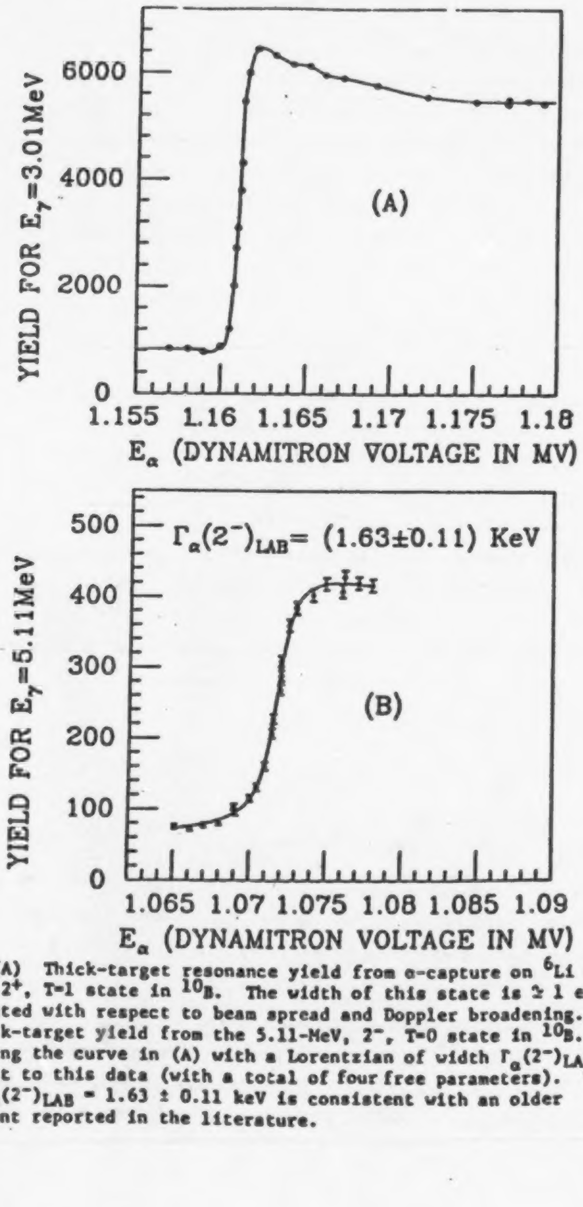

Fig. I-16. (A) Thick-target resonance yield from α-capture on ^{6}Li to the 5.16-MeV 2^+, T=1 state in ^{10}B. The width of this state is $\gtrsim$ 1 eV and can be neglected with respect to beam spread and Doppler broadening. (B) Thick-target yield from the 5.11-MeV, 2^-, T=0 state in ^{10}B. Integrating the curve in (A) with a Lorentzian of width $\Gamma_\alpha(2^-)_{LAB}$ yields a good fit to this data (with a total of four free parameters). The result $\Gamma_\alpha(2^-)_{LAB}$ = 1.63 ± 0.11 keV is consistent with an older measurement reported in the literature.

B. OPERATION OF THE DYNAMITRON FACILITY

The Physics Division operates a high-current 4.5-MV Dynamitron accelerator which has unique capability as a source of ionized beams of most atoms and many molecules. Among the unusual facilities associated with the Dynamitron are (1) a beam line capable of providing "supercollimated" ion beams permitting angular measurements to accuracies of 0.005 degree, (2) a beam-foil measurement system capable of measuring lifetimes down to a few tenths of a nanosecond, (3) an experimental system dedicated to measuring absolute nuclear cross sections at low energy, (4) a variety of experimental apparatus for weak-interaction studies, (5) a simultaneous irradiation system by which heavy ions from the Dynamitron and helium ions from a 2-MV Van de Graaff accelerator are focussed on the same target, (6) a post-acceleration chopper system giving beam pulses of variable width from about one nanosecond to the millisecond range at repetition rates variable up to 8 MHz, (7) a scattering chamber for electron spectroscopy with electrostatic parallel-plate electron spectrometers with variable energy resolution (0.1% to a 5%) and the capability to measure electron energies up to a few keV as a function of observation angle, and (8) a McPherson electrostatic spherical electron-spectrometer system capable of measuring electron energies with high precision and very high efficiency. A PDP-11/45 computer system is used for on-line data analysis and for the control of experiments.

1. OPERATIONAL EXPERIENCE

B. J. Zabransky, D. Schneider, R. L. Amrein, and A. E. Ruthenberg

Overall, the Dynamitron continued to perform well during the past year. The normal operating schedule was twenty-four hours a day, five days a week. Very little running was done on weekends during calendar year 1982.

During the year the accelerator was staffed a total of 5380 hours. Of this time 4729 hours (88%) were scheduled for experimental research during which a beam was provided to the experimenters 90% of the time. Machine preparation time used up 6% of the scheduled research time and machine malfunctions 4%. Scheduled accelerator improvements (including the upgrading program) and modifications used a total of 651 hours or 12% of the total available time.

The great versatility of the Dynamitron continued to be exploited by the research staff. Ion currents on target varied from less than a nanoampere to about 100 microamperes with ion energies ranging from 0.2 to 4.0 MeV. A wide range of both atomic and molecular ions was delivered on target. They included $^{1}H^{+}$, $^{1}H_2^{+}$, $^{2}H^{+}$, $^{1}H_3^{+}$, $^{3}He^{+}$, $^{2}H_2^{+}$, $^{4}He^{+}$, $^{4}HeH^{+}$, $^{2}H_3^{+}$, $^{7}Li^{+}$, $^{7}Li^{++}$, $^{7}Li^{+++}$, $^{12}C^{+}$, $^{14}N^{+}$, $^{14}N^{++}$, $^{20}Ne^{+}$, $^{20}Ne^{++}$, $^{14}N_2^{+}$, $^{40}Ar^{+}$, $^{40}Ar^{++}$, $^{40}Ar^{+++}$.

During the year a total of 55 investigators used the Dynamitron in some phase of their experimental research. Of these, 12 were from the Physics Division, 10 were from other Argonne research divisions, 21 were outside users from other research facilities, 9 were members of the Resident Graduate Student Program, and 3 were undergraduate students participating in research at the Dynamitron. Of the scheduled time, 89% went to experiments involving members of the Physics Division, 10% to other Argonne divisions, and 1% was exclusively assigned to outside users. However, outside users collaborated in experiments that used 66% of the total available time. Undergraduate students and participants in the Resident Graduate Student Program worked on experiments that used 77% of the time.

The accelerator has been heavily used by several research groups during 1982. It has been operating with only routine maintenance problems and relatively free of sparking for voltages up to 4 MV. Sparking above 4 MV is still a problem. The terminal control rods continue to be damaged even with special modifications. Early in 1983 the accelerator tube will be reoriented to try to correct this problem. A system to eliminate the control rods by the use of fiber-optic or infrared light-link control of stepping motors is being studied. Step-by-step improvements to the various machine components and configurations will be made as tests of the maximum energy-holding capability continue.

The fiber-optic light-link system for monitoring electrical parameters within the high-voltage terminal was damaged again by a series of sparks when the machine was operating in the 4-MV range. The fiber-optic bundle was removed to allow operation at higher energies. It will again be installed after being repaired and after the accelerator tube is reoriented. The bundle will be repositioned on the column so as to reduce damage.

Two beam lines were changed this year. One was built up to allow experiments using a McPherson electron spectrometer. A scattering chamber for electron spectroscopy was added to another beam line. The experimental area was improved with a large increase in the ambient light and a general organization of the area. Various vacuum improvements were made to several of the beam lines.

The development of ion sources to provide ion species of interest to specific experimental groups has proceeded slowly during the year because of the decrease in the number of technical staff. A beam of Li^+ can now be produced easilyand was used many times during the year. With only a minor modification, it is hoped that a Be^+ beam can be produced from the same source. A Penning source is being modified to accept cathodes made of Si in order to produce a Si^+ beam. The machining of the Si uses a special process and is being done by the Dynamitron technical staff.

A Capillaritron ion source is under development. It uses a nozzle with a 25-micron orifice. When gas flows through the nozzle and it is biased at 2 to 15 kV, a plasma forms just inside the tip, producing copious quantities of various ions. Initial tests are encouraging but many problems, including poor focussing and a high gas load on the accelerator tube, will have to be overcome.

2. UNIVERSITY USE OF THE DYNAMITRON

B. J. Zabransky

The Argonne Dynamitron continues to be a valuable research facility for scientists from outside institutions. It is not only the accelerator itself that attracts outside investigators but also the unique associated experimental equipment as well as the on-going research program being conducted at the Dynamitron.

Most visiting scientists chose to collaborate with local investigators on problems of common interest. A few, however, worked as an independent group. Some came for a one-time-only experiment, but most are participants in research programs that have spanned a period of several years.

During the year twenty-one scientists came from thirteen outside institutions to use the Dynamitron. They came from eight states and three foreign countries. They participated in experiments that used 66% of the time scheduled for research. A list of those institutions from which users of the Dynamitron came during 1982 is given below. The list includes the name of the institution, the title of the research project, and the names of the principal investigators. The names of their Argonne collaborators are enclosed in parentheses.

(1) Arizona State University
Development of Capillaritron Ion Source
J. Kelly, (D. S. Gemmell)

(2) University of Freiburg, Berlin, West Germany
Electron Spectroscopy of Fast-Ion Collisions
Using Simultaneous Laser Excitation
R. Bruch, (D. Schneider, W. Stöffler, V. Pfeufer,
B. Zabransky, H. G. Berry, and P. Arcuni)

(3) Fudan University, Shanghai, China
Influence of Rydberg States in Convoy Electron Measurements
Gu Yuan Zhuang, (D. S. Gemmell, E. P. Kanter,
D. Schneider, Z. Vager,* and B. J. Zabransky)

(4) Marquette University
Radiation Damage of Covalent Crystal Structures
L. Cartz, A. Gowda, F. G. Karioris,
and T. Ehlert

(5) Northwestern University
Direct Capture in the ^{27}Al(p,γ) and ^{19}F(p,γ) Reactions
R. E. Segel, E. Zupranska,* G. Hardie,* M. Wiescher,*
(A. J. Elwyn, and W. Ray)

(6) University of Notre Dame
Spectra of High Spin States in Light Elements
A. E. Livington, (H. G. Berry, J. Hardis, and W. Ray)

(7) Ohio State University
Direct Capture in the ^{27}Al(p,γ) and ^{19}F(p,γ) Reactions
M. Wiescher, G. Hardie,* R. E. Segel,* E. Zupranska,*
(A. J. Elwyn, and W. Ray)

(8) University of Texas
Autoionization Electron Spectroscopy of Li, He, Ne, and Ar
C. F. Moore, P. Seidel, (D. Schneider, P. Arcuni
and W. Stöffler)

(9) University of Toledo
Measurements of Forbidden Transition Rates
P. S. Ramanujam, L. Curtis, (H. G. Berry,
J. Hardis, and W. Ray)

(10) Valparaiso University
The ^{7}Li(d,p)^{8}Li Reaction and Solar Neutrino Capture Rates
D. Koetke, (B. Filippone, A. J. Elwyn, and W. Ray)

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*From another outside institution.

(11) Weizmann Institute, Rehovot, Israel
Studies of Beam-Foil Excited Rydberg Atoms
Z. Vager, (D. S. Gemmell, E. P. Kanter, D. Schneider, and B. J. Zabransky)

(12) Western Michigan University
Direct Capture in the ^{27}Al(p,γ) and ^{19}F(p,γ) Reactions
G. Hardie, R. E. Segel,* M. Wiescher,* E. Zupranska,* A. J. Elwyn, and W. Ray)

(13) Yale University
Microwave Field Ionization of Foil-Excited Fast Rydberg Atoms
P. Koch, D. Mariani, W. van de Water, (D. S. Gemmell, E. P. Kanter, D. Schneider, and B. J. Zabransky)

The Resident Graduate Student Program is open to students that have finished their course work and passed their prelims. They come to Argonne and perform their Ph.D. thesis research here. Nine members of this program worked at the Dynamitron during 1982. Altogether they participated in experiments that used 77% of the time allotted to research. Those who used the accelerator are listed below, together with their home university and their local thesis advisor.

(1) P. W. Arcuni, University of Chicago
H. G. Berry, advisor

(2) R. Evans, Iowa State University
C. N. Davids, advisor

(3) B. Filippone, University of Chicago
C. N. Davids, advisor

(4) M. Finn, University of Minnesota
C. N. Davids, advisor

(5) C. A. Gagliardi, Princeton University
G. T. Garvey, advisor

(6) J. Hardis, University of Chicago
H. G. Berry, advisor

(7) A. R. Heath, University of Chicago
G. T. Garvey, advisor

(8) W. Stöffler, Free University of Berlin
D. Schneider, advisor

(9) G. Zapalac, University of Chicago
H. G. Berry, advisor

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*From another outside institution.

In addition, the following undergraduate students have participated in research based at the Dynamitron.

(1) J. Bales, North Carolina State University
D. S. Gemmell, advisor

(2) J. J. Hofmann, East Stroudsburg State College
D. Schneider, advisor

(3) J. E. Tkaczyk, Rutgers University
E. P. Kanter, advisor

IX. BEAM-FOIL RESEARCH AND COLLISION DYNAMICS OF HEAVY IONS

Introduction

Our program consists of investigations of the structure and dynamics of atomic ions principally using photon detection techniques. The experiments involve fast ion beams produced at either the Tandem-Linac accelerator (30--300-MeV ion energy) or the Argonne Dynamitron accelerator (0.5--4.5-MeV ion energy) or a low energy "test-bench" facility (0.02--0.12-MeV ion energy). Laser excitation of the fast beams is anticipated in future experiments to study atomic structure principally of low ionization stages.

In 1982, the principal investigator, H. G. Berry, was in Europe until the end of July; part of the time was spent at the Aimé Cotton Laboratory, Orsay, France, learning laser techniques, and part of the time at the University of Lund doing beam-foil spectroscopy with a small Tandem accelerator.

The program at Argonne continued with a graduate student, Jon Hardis,* assisted by Professors A. E. Livingston† and L. J. Curtis‡ during their frequent visits to Argonne. This work involved two atomic structure problems in neon, plus a continuation of our study of electron channelplate geometries for more efficient data collection.

We have started our program of studies on the interactions of fast ion beams with lasers. An argon-ion pump laser and a CW ring dye laser with frequency-doubling capability have just been delivered. Initial experiments on collinear laser-fast ion beam resonant excitation are under construction.

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*Thesis student, University of Chicago, Chicago, IL.
†University of Notre Dame, Notre Dame, IN.
‡University of Toledo, Toledo, OH.

a. Lamb Shifts and Fine Structures of n = 2 in Helium-like Ions
(H. G. Berry and J. E. Hardis*)

Following our successful calculations and experiments in silicon, sulfur and chlorine of the $1s2s\,^3S_1 - 1s2p\,^3P_{0,2}$ transition wavelengths, we have continued this work in several directions:

(i) We are preparing a precision measurement in helium-like titanium of the same transition. An initial run is scheduled at the Argonne Tandem-Linac in early 1983. (See Fig. IX-1.)

(ii) A precision measurement in helium-like neon has been completed at the Argonne Dynamitron. This experiment involved the use of an

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*Thesis student, University of Chicago, Chicago, Illinois.

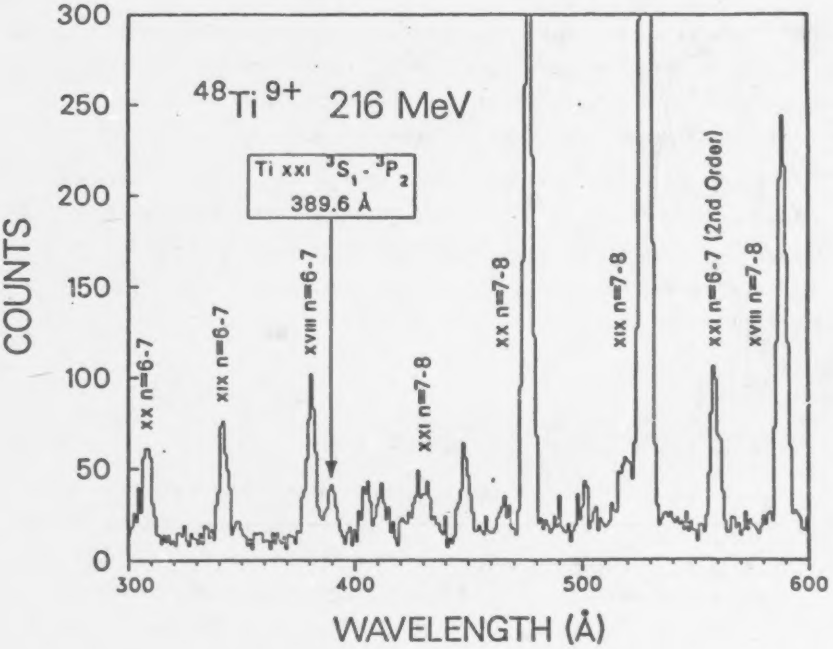

Fig. IX-1. Preliminary spectrum of 216-MeV titanium. The two-electron Ti XXI transition is noted.

8 MeV Ne^{2+} beam from the Dynamitron. The work should clarify some discrepancies in recent measurements from other laboratories on these transitions $1s2s\,^3S_1 - 1s2p\,^3P_{0,2}$ and give a useful test of our two-electron Lamb-shift calculations. The data are being analyzed.

(iii) We have improved our calculations of the total energies of the two states $1s2s\ ^3S$ and $1s2p\ ^3P$ for ions of low Z ($Z < 10$). We find significant discrepancies in some previously published results. A theoretical group at Oxford, England, (Grany et al.) have verified our earlier calculations for these energies at higher Z.

b. Precision Wavelength Measurements in Helium (H. G. Berry, P. Juncar,* H. T. Duong,* and R. Damaschini*)

In an experiment at Orsay, France, we have used saturated absorption spectroscopy and a sigmameter to obtain the absolute wavelengths of the $2p\ ^3P_{0,1,2} - 3d\ ^3D_{1,2,3}$ transitions near 587.6 nm in ^{4}He I. Our precision is about 8 parts in 10^9. By comparing with recent two-photon measurements of direct excitation from the $2s\ ^3S_1$ level, we obtain values for the wavelengths of the $2s\ ^3S_1 - 2p\ ^3P_{0,1,2}$ transitions. Precise calculations for these transitions are compared with experiment. In particular, we have analyzed the QED and relativistic corrections.

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*Laboratory of Aimé Cotton, Orsay, France.

c. Position-Sensitive Detector for UV Spectroscopy (J. E. Hardis* and H. G. Berry)

We continue to investigate designs of one-dimensional position-sensitive detectors for the exit focus of our UV spectrometer. A microchannel plate (MCP) serves as a front-end photon detector and signal amplifier. Techniques for imaging the output electron signal of the MCP are under study. Nonlinearities and drift in carbon-resistive-anode readouts limit theprecision of the effective spectral dispersion curve obtained. Conductive wedges appear to hold promise, and computer modeling is underway. Application of digital VLSI technology and multi-anode techniques are also under review.

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*Thesis student, University of Chicago, Chicago, IL.

d. High-spin States in Neon (J. E. Hardis,* A. E. Livingston,† L. J. Curtis,‡ and H. G. Berry)

Past experiments in this laboratory have identified the quartet ($1s2s2p\ ^4P^o - 1s2p^2\ ^4P$) and quintet ($1s2s2p^2\ ^5P - 1s2p^3\ ^5S$) transitions in carbon, nitrogen, and oxygen. Higher beam energies at the Dynamitron, needed to excite the same doubly-excited states in heavier elements, were not available. We have now a good source (2--3 μA) of doubly-charged neon for the Dynamitron accelerator. This effectively doubles the terminal voltage for that projectile. The quartet spectral lines have been located, and measurements of their wavelengths and lifetimes have been completed.

The quintet states have been identified and measurements of their wavelengths and lifetimes are in progress.

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†University of Notre Dame, Notre Dame, IN.

‡University of Toledo, Toledo, OH.

e. Multicharged Ions at the Dynamitron (J. E. Hardis,* R. Amrein, W. Ray and H. G. Berry)

In addition to upgrading the Dynamitron terminal voltage, we have attempted to increase the energy of certain beams by producing multicharged ions directly at the ion source. Tests with a Penning ion source have thus far been disappointing. However, by careful adjustment of gas pressures and mixtures (e.g., of Ne and H_2), an rf ion source has given reasonable quantities of well-focussed beams of Ne^{2+} and Ar^{n+} with n = 2, 3, and 5. Other rare gas ions should also be feasible. Addition of a crossed-field analyzer at the source is expected to purify the higher charged beams.

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*Thesis student, University of Chicago, Chicago, Illinois.

f. Measurement of the Transition Probability of Singlet-Triplet Intercombination Lines in Neon (L. J. Curtis*, J. E. Hardis†, R. L. Brooks and A. E. Livingston‡)

Using the same doubly-charged neon beam mentioned above, we have measured the lifetimes of the neon $1s^22s3p\ ^3P_{0,1,2}$ states. The J = 1 state has only about half the lifetime of the other two, and this difference is attributed to the extra decay channel to the $1s^22s^2\ ^1S_0$ state, accessible to it alone. The smaller value for J = 1 is due to a J-allowed decay channel to $2s^2\ ^1S_0$, and implies a transition probability of $4.3(6) \times 10^8$ sec^{-1} for this intercombination line. These measurements extend similar measurement of lighter elements done previously at lower energies (at Lund, Sweden). This purely relativistic phenomenon is more pronounced in neon than in the lighter elements.

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‡University of Notre Dame, Notre Dame, IN.

g. Optical Measurements of Molecular-Ion Fragmentation (H. G. Berry, L. Engström,* S. Huldt,* and I. Martinson*)

In an experiment in Lund, Sweden, we observed the break-up of fast CN^+ ions in thin carbon foils. CN^- was accelerated in a 3-MV Pelletron Tandem accelerator and charge-exchanged to CN^+ at the center gas stripper to produce, typically, 100 nA of 5-MeV CN^+ ions on target. Light yields from several transitions in high ionization stages of C and N were observed to vary as a function of carbon foil thickness. For very thin foils the neighboring fragment ion is close enough to influence and enhance the excited state production in these ions. The work is continuing both at Argonne and at Lund. (See Fig. IX-2.)

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*University of Lund, Sweden.

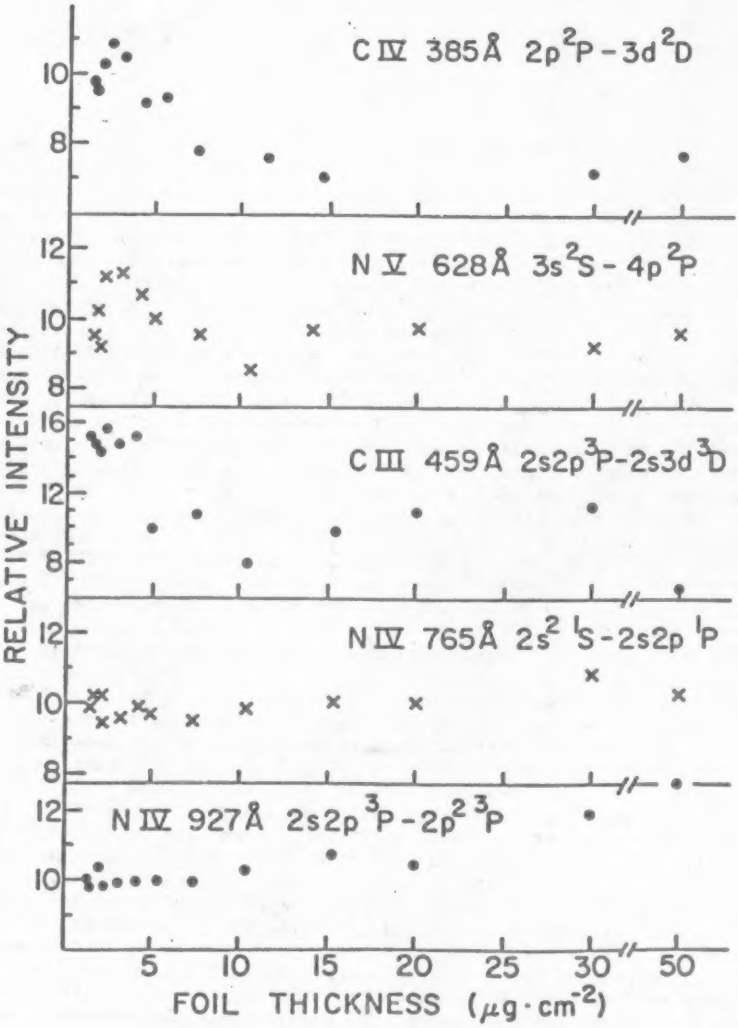

Fig. IX-2. Carbon-foil thickness dependence of carbon-ion and nitrogen-ion light yields for 5-MeV incident CN^+ molecular ions.

X. INTERACTIONS OF FAST ATOMIC AND MOLECULAR IONS WITH SOLID AND GASEOUS TARGETS

Introduction

Tightly collimated beams of molecular ions with energies variable in the range 0.5--4.5 MeV are directed onto thin (~100 Å) foil or gaseous targets. The distributions in energy and angle are measured with high resolution (~0.005° and ~300 eV) for the resultant collisionally-induced dissociation fragments. The major aim of the work is a general study of the interactions of fast ions with matter, but with emphasis on those aspects unique to the use of molecular-ion projectiles. In addition, we are able to study of the structures of the incident molecular ions. These two different aspects of the work are mutually interdependent. In order to derive structure information about a given molecular ion, one needs to know details about the way the dissociation fragments collectively interact with the target in which the dissociation occurs. Similarly, a knowledge of the structure of the incident molecular clusters is important in understanding the physics of their interactions with the target. We have therefore begun our work with careful studies involving beams of the simplest and relatively well understood diatomic molecular ions (H_2^+, HeH^+, etc.). Even with these, several new and interesting phenomena have been encountered (e.g., the interactions between the molecular constituents and the polarization oscillations that they induce in a solid target, the marked differences in dissociations induced in gases as compared with those in foils, the anomalously high transmission of some molecular ions through foils, and striking electron capture phenomena when compared to atomic ions). As our understanding of these phenomena develops, we plan to go on to studies involving ever more complex projectile ions.

In the course of developing techniques for determining the stereochemical structures of molecular projectiles by coincident detection of dissociation fragments, preliminary data have shown us the important problems which need to be addressed in order to obtain precise structural information. Most prominently, these problems include the need for a more detailed understanding of the physical processes involved in the interactions of these fast molecular ions with solid targets and the formation of final electronic states. This year we concentrated our efforts on studying the formation of high Rydberg atoms when fast ions exit solids. These atoms were found to emerge with high probability when fast molecular-ion beams dissociate in foils. Our work was aimed at understanding the processes which lead to the formation of these atoms. Also this year, we demonstrated that K-vacancy equilibration lengths for fast ions traversing solids are much longer than previously anticipated. This was an important confirmation of our model for the observed charge-state dependence of angular multiple-scattering widths for such ions.

Some of the highlights in 1982 included:

a. Contribution of Field-Ionized Rydberg Atoms to Convoy Electron Spectra (D. S. Gemmell, Y.-Z. Gu, E. P. Kanter, D. Schneider, Z. Vager, and B. J. Zabransky)

A prominent feature observed in the energy spectrum of electrons emitted in the forward direction from thin foils and gas targets under bombardment by fast ions is a sharp cusp-shaped peak occurring at an energy where the electron velocity matches the velocity of the emerging projectile ions. For fast light ions, these "cusp" electrons were believed to originate from the capture of target electrons into projectile-centered continuum states. Intense experimental and theoretical efforts have been directed towards understanding the measured cusps in terms of various theories of this so-called electron-capture-to-the-continuum (ECC) model, as well as a competing "wake-riding" model. To date, none of these various theoretical treatments has had any success in explaining the full range of experimental data now available from cusp-electron measurements. In pursuing our efforts to explain some puzzling features of molecular-ion dissociation experiments which had suggested the production of large numbers of high Rydberg atoms in fast beams, we have also tried to determine the extent to which the presence of significant numbers of such atoms could be affecting observations of cusp electrons.

If electron capture can occur into continuum states lying just above the ionization threshold of the projectile, there seems to be no *a priori* reason why capture into bound states lying just below the ionization threshold cannot also occur with comparable probability. The fate of Rydberg atoms emerging from a target can be expected to depend sensitively, and in ways difficult to predict, upon details of the experimental apparatus. Rydberg atoms have long radiative lifetimes, but they can be ionized in quite modest electric fields. Certainly the electric fields used in most electron spectrometers suffice to ionize a large fraction of Rydberg atoms entering the spectrometer. Because it is customary in measurements of cusp electrons to pass the projectiles emerging from the target through a spectrometer, it is likely that field-ionizing Rydberg atoms will contribute electrons, traveling with the beam velocity, to the secondary electron spectrum.

In our initial experiments, we incorporated a deflecting field intermediate between the target and electron spectrometer. By jointly sweeping the voltages on the deflecting plates, and the electron spectrometer, we found that although electrons emerging from the target were eliminated as anticipated by the deflecting field, there existed a sizable contribution of beam-velocity electrons which originated after the deflecting field. Further measurements with a +60 volt bias on the foil target shifted the cusp electrons to lower energy and allowed a separation of the target "cusp" from the field-ionizing Rydberg contribution.

We have further studied the systematics of this phenomenon with various ion beams (both atomic and molecular), targets, beam energies, and experimental geometries. Quite recently, we extended these measurements to include highly energetic heavy-ion beams. Using the Argonne Tandem-Linac heavy-ion accelerator, we studied the field ionization of high Rydberg ($n > 300$) sulphur ions produced by beam-foil excitation of a 125-MeV sulphur beam. That experiment conclusively demonstrated a very high yield of such atoms as had been suspected from previous studies of the delayed x-ray emission of these fast heavy ions.

These measurements, demonstrating the large yield of Rydberg atoms formed in excited fast ion beams, have far-reaching consequences in several areas of atomic collision physics. Most importantly, many measurements of charge-state yields and charge-changing cross sections must be reinvestigated in the light of this discovery.

b. Microwave Field Ionization of Fast Rydberg Atoms (P. Arcuni,* D. S. Gemmell, E. P. Kanter, P. M. Koch,† D. R. Mariani,† D. Schneider, W. van de Water,† and B. J. Zabransky)

In an attempt to determine the quantum-state populations for beam-foil excited high Rydberg atoms, we have collaborated with a group from Yale University in studying the microwave ionization of such atoms. We used a

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†Yale University, New Haven, Connecticut.

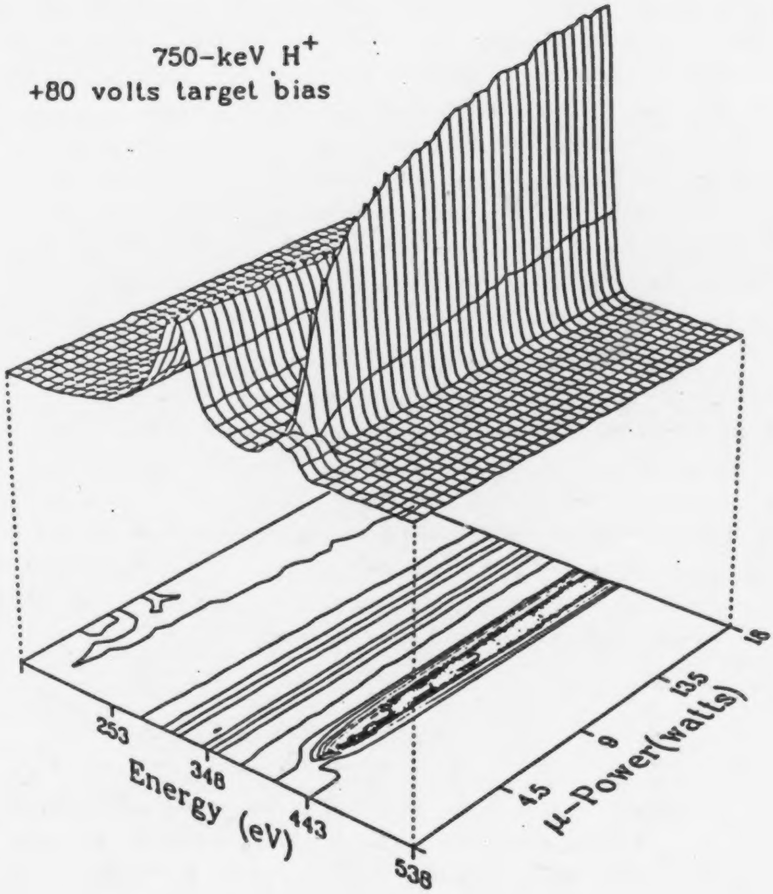

Fig. X-1. A joint distribution of 0° electrons showing energy spectra for various levels of microwave power (watts). The lower-energy peak, unaffected by microwave power, is caused by convoy electrons. The higher-energy peak, which grows with power, is produced by field-ionization of Rydberg atoms in the microwave cavity. At lower power, there is an additional contribution from atoms ionizing in the spectrometer field (170 v/cm).

9.91-GHz microwave cavity to ionize Rydberg atoms after production in a thin carbon foil, but before entering the electron spectrometer field used to energy-analyze the resulting electrons. Because of its high frequency, the variable microwave electric field had only a negligible effect on the energy spectrum of electrons originating prior to the cavity. By applying a bias voltage to the foil target, we were able to separate clearly those electrons produced at the target from those created in the cavity. An additional contribution was observed from field ionization in the spectrometer field when the microwave field was reduced below the magnitude of that field. (See Fig. X-1.)

This experimental geometry separates the ionizing field from the analyzing field, allowing us to vary the former to much higher values than we had been able to achieve before. With a microwave power of 18.4 watts, we achieved a maximum electric field of about 2.8 kV/cm which would ionize hydrogen atoms as low as n = 24. Analysis of the data so far seems to indicate that the n population is consistent with a simple OBK-type last-layer capture process. It is hoped that a better understanding of the microwave ionization process will yield more detailed information about the distribution of kinetic energy of the electrons that we observe.

c. Coherent Stark States in Foil-Excited Fast Rydberg Atoms

(D. S. Gemmell, E. P. Kanter, D. Schneider, and Z. Vager)

In a further effort to determine the quantum-state population of foil-excited fast Rydberg atoms, we studied the field ionization of these atoms in a variety of field geometries. One finding is that transverse electric fields are more effective in ionizing such atoms than are longitudinal fields. This is a strong indication of high alignment in the excitation and suggests an electron density in these states which is oblate with respect to the beam direction. A very surprising finding was the observation of oscillations in the ionization yield when a longitudinal electric field, starting at the target, is varied in magnitude. (See Fig. X-2.) These oscillations are regularly spaced, with a period that varies with the beam energy. We have demonstrated that these observations imply coherent excitation of a few Stark levels near the unshifted center of the Stark

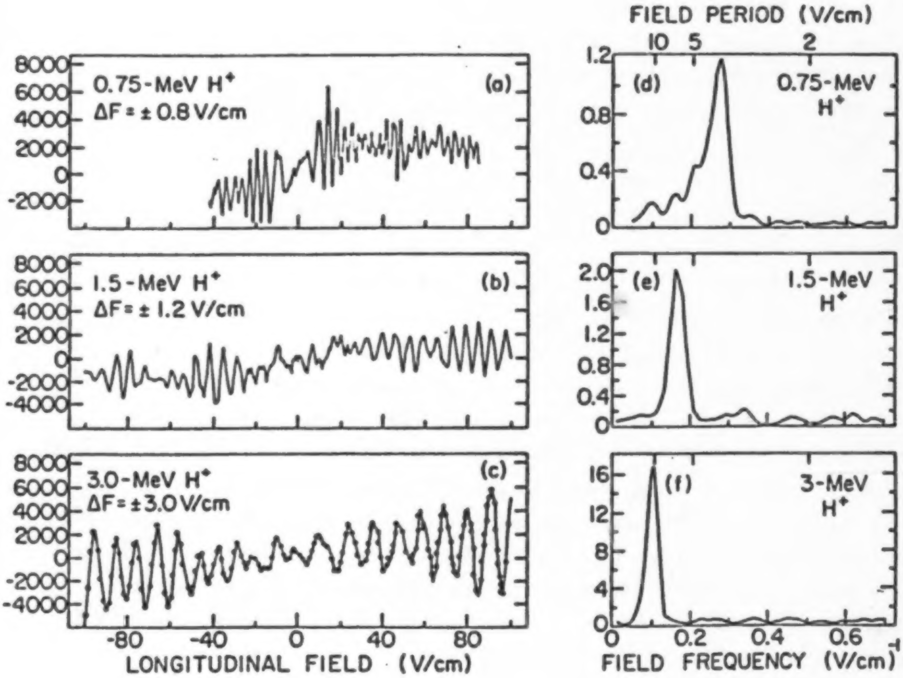

Fig. X-2. A comparison of differential yield curves as a function of longitudinal field for three different proton bombarding energies, (a) 0.75 MeV, (b) 1.5 MeV, and (c) 3 MeV, in the region between ±100 V/cm. The square-wave fields, ±ΔF, are shown in each. The Fourier power spectrum for each energy is shown in (d), (e), and (f), respectively. The Fourier spectra are computed from the full range of data measured for each energy.

manifold. The observed modulations are extremely sensitive to the amplitudes of the coherently excited states. This phenomenon offers a new and potentially powerful technique for studying excitation mechanisms that produce high Rydberg states of fast projectiles as they exit solids.

d. Equilibration Lengths of K-Vacancy Production in Solids
(E. P. Kanter, D. Schneider, and B. J. Zabransky)

Measurements on the angular distributions of fast ions traversing foils have shown a pronounced dependence of the multiple-scattering widths upon the charge state of the emerging ions. We have successfully explained these results in terms of the large scattering angles achieved by those ions that bear K vacancies. A quantitative model has been developed which demonstrates how the "memory" of K-vacancy producing collisions gives rise to large multiple-scattering widths in spite of apparent charge-state equilibration. The K-shell capture and loss cross sections are an important input to this model. Because these cross sections are largely unknown, we have conducted a series of experiments to determine the K-shell charge-exchange equilibration lengths for fast ions in foils. By measuring the yield of KLL Auger electrons from 0.4- and 2.7-MeV N^+ ions exiting solid carbon targets, we have demonstrated that indeed the K-equilibration lengths are longer than had been previously assumed, confirming our model of the multiple-scattering data.

e. Analysis of Molecular-Ion Stopping Power Measurements
(D. S. Gemmell, E. Johnson,* E. P. Kanter, and M. F. Steuer)

Following the discovery in 1974 of the influence of cluster effects upon the slowing down of ions in solids, there have been several experimental and theoretical investigations of this phenomenon. In general, the cluster stopping powers for light projectiles such as H_2^+ are fairly well described on the basis of wake models derived from Lindhard's dielectric function. The situation for heavy clusters, however, appears to be more complex.

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*Graduate student, Oxford University, England.

We have measured the stopping power ratio of N^+ fragments from equal velocity beams of N^+ and N_2^+. In contrast with the earlier work on light ions, we were able to select molecular N^+ fragment pairs that were "longitudinally" aligned to the beam direction upon exiting the foil. This orientational selectivity greatly simplifies the analysis.

Surprisingly, the results show that, contrary to the light ion data, the stopping power of heavy molecular clusters is diminished relative to of the corresponding monatomic projectiles. This implies that most of the induced negative polarization charge must lie between the separating fragment ions.

An intense effort to explain these data has yielded only limited success. We have learned that it is vital to use a non linear wake model for such heavy diatomic ions. To avoid the complexities of a proper quantum-mechanical treatment we have employed a semiclassical calculation of free-electron scattering by two screened ionic cores to compute the stopping forces as the ions traverse the solid. This method has had success in describing our highest energy (3-MeV) stopping data, however, several problems limit the applicability of this approach.

PUBLICATIONS FROM 1 APRIL 1982 THROUGH 31 MARCH 198

The list of "journal articles and book chapters," is classified by topic; the arrangement is approximately that followed in the Table of Contents of this *Annual Review*. The "reports at meetings" include abstracts, summaries, and full texts in volumes of proceedings; they are listed chronologically.

A. JOURNAL ARTICLES AND BOOK CHAPTERS

Isospin Effects in Pion Single-Charge-Exchange Reactions
D. Ashery, D. F. Geesaman, R. J. Holt, H. E. Jackson, J. R. Specht, K. E. Stephenson, R. E. Segel (Northwestern), P. Zupranski (Northwestern), H. W. Baer (LANL), J. D. Bowman (LANL), M. D. Cooper (LANL), M. Leitch (LANL), A. Erel (Tel Aviv. U.), R. Chefetz (Tel Aviv U.), J. Comuzzi (MIT), R. P. Redwine (MIT), and D. R. Tieger (Boston U.)
Phys. Rev. Lett. 50, 482, (1983)

Isospin Splitting of the Giant Dipole Resonance in ^{60}Ni
T. J. Bowles, R. J. Holt, H. E. Jackson, R. D. McKeown, A. M. Nathan (U. Illinois), and J. R. Specht
Phys. Rev. Lett. 48, 986 (1982)

Erratum: Isovector Radiavie Decays and Second-Class Currents in Mass 8 Nuclei [Phys. Rev. C 18, 1447 (1978)]
T. J. Bowles and G. T. Garvey
Phys. Rev. C 26, 2336 (1982)

Measurement of the ^{7}Be(p,γ)^{8}B Reaction Cross Section at Low Energies
B. W. Filippone, A. J. Elwyn, C. N. Davids, and D. D. Koetke (Valparaiso U.)
Phys. Rev. Lett. 50, 412 (1983)

Demonstration of the Need for Meson Exchange Currents in the Beta Decay of ^{16}N(0$^-$)
C. A. Gagliardi, G. T. Garvey, J. R. Wrobel, and S. J. Freedman (Stanford U.)
Phys. Rev. Lett. 48, 914 (1982)

Erratum: Beta-Alpha Angular Correlations in Mass 8 [Phys. Rev. C 22, 738 (1980)]
R. D. McKeown, G. T. Garvey, and C. A. Gagliardi
Phys. Rev. C 26, 2336 (1982)

Observation of the (π^-,π^-n) and (π^+,π^+p) Reactions at 165 MeV
E. Piasetsky (Tel Aviv U.), A. Altman (Tel Aviv U.), J. Lichtenstadt (Tel Aviv U.), A. I. Yavin (Tel Aviv U.), D. Ashery, W. Bertl (ETH, Zurich), L. Felawka (ETH, Zurich), H. K. Walter (ETH, Zurich), F. W. Schlepütz (U. Zurich), R. J. Powers (U. Zurich), R. G. Winter (U. Zurich and C. of Wm. and Mary), and J. v. d. Pluym (Vrije U., Amsterdam)
Phys. Lett. 114B, 414 (1982)

Pion-Induced Nucleon Knockout Reactions on ^{16}O and ^{18}O
E. Piasetzky (Tel Aviv U.), A. Altman (Tel Aviv U.), J. Lichtenstadt (Tel Aviv U.), A. I. Yavin (Tel Aviv U.), D. Ashery, W. Bertl (ETH, Zurich), L. Felawka (ETH, Zurich), H. K. Walter (ETH, Zurich), F. W. Schlepütz (U. Zurich), R. J. Powers (U. Zurich), R. G. Winter (U. Zurich and C. of Wm. and Mary), and J. v. d. Pluym (Vrije U., Amsterdam)
Phys. Rev. C 26, 2702 (1982)

Study of the ^{39,41}K(d,^{3}He)^{38,40}Ar Reactions at 22.8 MeV
C. M. Bhat (Bangalore U., India), M. Raja Rao (Bangalore U.), N. G. Puttaswamy (Bangalore U.), and J. L. Yntema
Nucl. Phys. A394, 109 (1983)

^{7}Li(d,p)^{8}Li Reaction Cross Section Near 0.78 MeV
A. J. Elwyn, R. E. Holland, C. N. Davids, and W. Ray, Jr.
Phys. Rev. C 25, 2168 (1982)

Absolute Cross Section for ^{7}Li(d,p)^{8}Li and Solar Neutrino Capture Rates
B. W. Filippone, A. J. Elwyn, W. Ray, Jr., and D. D. Koetke (Valparaiso U., Indiana)
Phys. Rev. C 25, 2174 (1982)

γ Decay of States in ^{47}Cr
G. Hardie (Western Mich. U., Kalamazoo, MI), S. A. Gronemeyer, L. Meyer-Schützmeister, and A. J. Elwyn
Phys. Rev. C 26, 456 (1982)

^{180}Ta^{g,m} Production Cross Sections from the ^{180}Hf(p,n) Reaction
Eric B. Norman, Timothy R. Renner, and Patrick J. Grant (U. Washington, Seattle, WA)
Phys. Rev. C 26, 435 (1982)

Prompt Compound Nuclear K x Rays in Fusion Reactions Induced by a Heavy Projectile
H. Ernst, W. Henning, C. N. Davids, W. S. Freeman, T. J. Humanic, M. Paul, S. J. Sanders, F. W. Prosser, Jr. (U. Kansas), and R. A. Racca (U. Kansas)
Phys. Lett 119B, 307 (1982)

Search for Transient Electric Field Gradients Acting on Fast-Moving Ions in Solids
H. Ernst, W. Henning, T. J. Humanic, T. L. Khoo, Steven C. Pieper, and J. P. Schiffer
Phys. Rev. C 26, 2039 (1982)

Reactions to Resolved States and to Non-fusion Channels for ^{16}O + ^{48}Ca at E_{lab} = 158.2 MeV
T. J. Humanic, H. Ernst, W. Henning, and B. Zeidman
Phys. Rev. C 26, 993 (1982)

Nuclear Radiation
Dennis G. Kovar
McGraw-Hill Encyclopedia of Science and Technology, 5th edition, ed. by S. P. Parker (McGraw-Hill, NY, 1982), pp. 320-321

Nuclear Reaction
Dennis G. Kovar
McGraw-Hill Encyclopedia of Science and Technology, 5th edition, ed. by S. P. Parker (McGraw-Hill, NY, 1982), pp. 322-326

Inelastic Scattering and One-Neutron-Transfer Reactions of ^{18}O + ^{40}Ca
K. E. Rehm, W. Henning, J. R. Erskine, and D. G. Kovar
Phys. Rev. C 26, 1010 (1982)

Inelastic Scattering of ^{16}O from ^{40,42,44,48}Ca
K. E. Rehm, W. Henning, J. R. Erskine, D. G. Kovar, M. H. Macfarlane, S. C. Pieper, and M. Rhoades-Brown
Phys. Rev. C 25, 1915 (1982)

Strong Population of Excited 0^+ States in Even Zr Isotopes Observed with the (^{14}C,^{16}O) Reaction
Wolfgang Mayer (Technische Universität Munchen, Garching, W. Germany), D. Pereira (TUM, Germany), K. E. Rehm (TUM, Germany), H. J. Scheerer (TUM, Germany), H.J. Körner (TUM, Germany), G. Korschinek (TUM, Germany), Waltraud Mayer (TUM, Germany), P. Sperr (TUM, Germany), Steven C. Pieper, and R. D. Lawson
Phys. Rev. C 26, 500 (1982)

High Spin States in ^{94}Ru and ^{95}Rh
A. Amusa (PHY/U. Ife) and R. D. Lawson
Z. Phys. A 307, 333 (1982)

Relativistic Quantum Mechanics of Particles with Direct Interactions
F. Coester and W. N. Polyzou (MIT)
Phys. Rev. D 26, 1348 (1982)

Coherence, Mixing, and Interference Phenomena in Radiative ψ Decays
Isaac Cohen (Weizmann Inst., Israel), Nathan Isgur (U. Toronto), and Harry J. Lipkin
Phys. Rev. Lett. 48, 1074 (1982)

Isospin Dependence of Pion Absorption on ^{3}He
T.-S. H. Lee and K. Ohta (MIT, Cambridge)
Phys. Rev. Lett. 49, 1079 (1982)

Microscopic Study of the Δ-Nucleus Potential from a Many-Body Hamiltonian for π, N and Δ
T.-S. H. Lee and K. Ohta (MIT, Cambridge)
Phys. Rev. C 25, 3043 (1982)

Angular Momentum Paradoxes with Solenoids and Monopoles
Harry J. Lipkin and Murray Peshkin
Phys. Lett. 118B, 385 (1982)

Isotope Targets Prepared by Vapor Deposition
G. E. Thomas
Nucl. Instrum. Methods 200, 27 (1982)

High Intensity Inverted Sputter Source
J. L. Yntema and P. J. Billquist
Nucl. Instrum. Methods 199, 637 (1982)

Yrast $(\pi h_{11/2})^n$ Excitations in Proton-Rich N=82 Nuclei
H. Helppi (Purdue U.), Y. H. Chung (Purdue U.), P. J. Daly (Purdue U.), S. .R. Faber (Purude U.), A. Pakkanen (Purdue U.), I. Ahmad (CHM), P.Chowdhury, Z. W. Grabowski, T. L. Khoo, R. D. Lawson, and J. Blomqvist (Res. Inst. Phys., Stockholm)
Phys. Lett. 115B, 11 (1982)

Transition from Collective to Aligned-Particle Configurations at High Spin in ^{154}Dy
A. Pakkanen (Purdue U.), Y. H. Chung (Purdue U.), P. J. Daly (Purdue U.), S. R. Faber (Purdue U.), H. Helppi (Purdue U.), J. Wilson (Purdue U.), P. Chowdhury, T. L. Khoo, I. Ahmad (CHM), J. Borggreen, Z. W. Grabowski, and D. C. Radford (Yale U.)
Phys. Rev. Lett. 48, 1530 (1982)

Search for Structure in the Fusion of ^{16}O + ^{24}Mg
R. A. Racca (U. of Kansas), F. W. Prosser (U. of Kansas), C. N. Davids, and D. G. Kovar
Phys. Rev. C 26, 2022 (1982)

Photoionization Mass Spectrometry of NH_2OH: Heats of Formation of HNO^+ and NOH^+
R. E. Kutina, G. L. Goodman and J. Berkowitz
J. Chem. Phys. 77, 1664-1676 (15 Aug. 1982)

Photoionization Mass Spectrometry of CH_3SH, CD_3SH and CH_3SD: Heats of Formation of $CH_3S^+(CH_2SH^+)$, CH_2S^+, CH_2S and HCS^+
R. E. Kutina, A. K. Edwards, G. L. Goodman and J. Berkowitz
J. Chem. Phys. 77, 5508-5526 (1 Dec. 1982)

Hyperfine Structure of the X $^2\Sigma$ Ground State of Ca^{35}Cl and Ca^{37}Cl by Molecular-Beam Laser-rf Double Resonance
W. J. Childs, David R. Cok, and L. S. Goodman
J. Chem. Phys. 76, 3993-3998 (15 April 1982)

Hyperfine Structure of the A $^2\pi$ State of Ca^{35}Cl
W. J. Childs, David R. Cok, and L. S. Goodman
J. Opt. Soc. Am. 72, 717-719 (June 1982)

Vibrational, Rotational, and Isotopic Dependence of CaBr X $^2\Sigma$ Spin-Rotational and hfs Parameters
W. J. Childs, David R. Cok, and L. S. Goodman
J. Mol. Spectrosc. 95, 153-156 (1982)

New Line Classifications in Ho I Based on High-Precision Hyperfine-Structure Measurement of Low Levels
W. J. Childs, David R. Cok, and L. S. Goodman
J. Opt. Soc. Am. 73, 151 (1983)

Doubly Excited States in Some Light Atoms
H. Gordon Berry, Robert L. Brooks, Jonathan E. Hardis, and W. J. Ray
Nucl. Instrum. Methods 202, 73-77 (1982)

Comparisons Between Theory and Experiment in Two Electron Systems
H. G. Berry, R. DeSerio and R. L. Brooks
Nucl. Instrum. and Methods 202, 95-101 (1982)

Beam-Foil Spectroscopy
H. G. Berry and M. Hass (Weizman Inst., Rehovot, Israel)
Ann. Rev. Nucl. Part. Sci. 32, 1-34 (1982)

Hyperfine Structures of the nd $^1D(n = 3\text{--}8)$ States of ^{3}He I
Robert L. Brooks, Vincent F. Streif and H. Gordon Berry
Nucl. Instrum. Methods 202, 113-117 (1982)

Alignment and Orientation of the 3p ^3P He I Term After Tilted-Foil Excitation
R. L. Brooks, H. G. Berry and E. H. Pinnington (Univ. of Alberta, Edmonton, Alberta, Canada)
Phys. Rev. A 25, 2545-2549 (1982)

Measurement of the Transition Probability of the $2s^2\ {}^1S_0\text{-}2s3p\ {}^3P_1^0$ Intercombination Line in Ne VII
J. E. Hardis, L. J. Curtis, P. S. Ramunujam, A. E. Livingston, and R. L. Brooks
Phys. Rev. A27, 257--261 (January 1983)

Spectroscopie et Mesures de Vies Moyennes de Niveaux de Nickel Hautement Ionise
C. Jacques (Universite Laval, Quebec, Canada), M. Druetta (Universite de Lyon, Villeurbanne, France), H. G. Berry and E. J. Knystautas (Universite Laval, Quebec, Canada)
Nucl. Instrum. Methods 202, 45-47 (1982)

Energies of Some Triplet Levels in ^{4}He I
P. Juncar (Lab. Aime Cotton, France), H. G. Berry, R. Damaschini (Lab. Aime Cotton), and H. T. Duong (Lab. Aime Cotton)
J.Phys. B: At. Mol. Phys. 16, 381 (1983)

Collisional Effects in the Passage of Fast Molecular Ions Through Thin Foils

Donald S. Gemmell

Nucl. Instrum. Methods 194, 255 (1982)

Ion-Source Dependence of the Distributions of Internuclear Separations in 2-MeV HeH^+ Beams

Elliot P. Kanter, Donald S. Gemmell, Itzhak Plesser, and Zeev Vager

Nucl. Instrum. Methods 194, 307 (1982)

Diminished Stopping Power for Fast Nitrogen and Oxygen Diclusters in Carbon

Malcolm F. Steuer, Donald S. Gemmell, Elliot P. Kanter, Edward A. Johnson, and Bruce J. Zabransky

Nucl. Instrum. Methods 194, 277 (1982)

Influence of Increasing Nuclear Charge on the Rydberg Spectra of Xe, Cs^+ and Ba^{++}: Correlation Term Dependence, and Autoionization

W. T. Hill III (NBS), K. T. Cheng, W. R. Johnson (U. of Notre Dame), T. B. Lucatorto (NBS), T. J. McIlrath (U. Maryland), and J. Sugar (NBS)

Phys. Rev. Lett. 49, 1631 (1982).

Correlation and Relativistic Effects in Spin-Orbit Splittings

K.-N. Huang (RER), Y.-K. Kim (RER), K. T. Cheng, and J. P. Desclaux (Grenoble)

Phys. Rev. Lett 48, 1245 (1982).

Target-Thickness Dependence of K-Shell Vacancy Fractons in Foil-Excited Ion Beams

D. Schneider, E. P. Kanter, and B. J. Zabransky

Phys. Rev. A 26, 3700-3701 (1982)

B. PUBLISHED REPORTS AT MEETINGS

Proceedings of the International School of Physics "Enrico Fermi", Varenna, Italy, 23 June-5 July 1980.

Brueckner-Bethe Calculations of Nuclear Matter
B. D. Day
Course LXXIX ed. by A. Molinari (North-Holland, Amsterdam, 1981), pp. 1-71

Proceedings of the Netherlands Physical Society 1980 International Summer School on Nuclear Structure, Dronten, The Netherlands, 12-23 August 1980.

Nuclear Structure and Heavy-Ion Reactions
John P. Schiffer
Ed. by K. Abrahams, K. Allaart, and A. E. L. Dieperink (Plenum, NY, 1981), pp. 127-163

Proceedings of the Ninth World Conference of the International Nuclear Target Development Society, Gatlinburg, Tennessee, 13-16 October 1980

Isotope Targets Prepared by Vapor Deposition
G. E. Thomas
Ed. by E. H. Kobisk and H. L. Adair (North-Holland, 1982), pp. 27-31 [Reprinted from Nucl. Instrum. Methods 200, 27 (1982)]

Proceedings of the Sixth International Conference on Fast Ion Beam Spectroscopy, Laval, Quebec, Canada, 17-20 August 1981

Doubly Excited States in Some Light Atoms
H. Gordon Berry, Robert L. Brooks, Jonathan E. Hardis, and W. J. Ray
Ed. by E. J. Knystautas and R. Drouin (North-Holland, 1982) +Nucl. Instrum. Methods 202, 73 (1982)

Comparisons Between Theory and Experiment in Two Electron Systems
H. G. Berry, R. DeSerio, and R. L. Brooks
Ed. by E. J. Kynstautas and R. Drouin (North-Holland, 1982) +Nucl. Instrum. Methods 202, 95-101 (1982)

Hyperfine Structures of the nd $^1D(n = 3\text{—}8)$ States of ^{3}He I
Robert L. Brooks, Vincent F. Streif, and H. Gordon Berry
Ed. by E. J. Kynstautas and R. Drouin (North-Holland, 1982)
+Nucl. Instrum. Methods 202, 113 (1982)

Spectroscopie et Mesures de Vies Moyennes de Niveaux de Nickel Hautement Ionise
C. Jacques (U. of Laval, Quebec), M. Druetta (U. of Lyon, France), H. G. Berry, and E. J. Knystautas (U. Laval)
Ed. by E. J. Kynstautas and R. Drouin (North-Holland, 1982)
+Nucl. Instrum. Methods 202, 45 (1982)

Proceedings of the 1981 Annual Meeting of the Optical Society of America, Kissimmee, Florida, 26-30 October 1981

Photoionization of Atoms and Molecules
J. Berkowitz
J. Opt. Soc. Am. 71, 1579 (1981)

Proceedings of the U.S.-Japan Seminar on Charged-Particle Penetration Phenomena, Honolulu, Hawaii, 25-29 January 1982

"Interactions of Fast Molecular Ions Traversing Thin Foils" - "The Contribution from Field-Ionized Rydberg Atoms in Measurements on Convoy Electrons"
Donald S. Gemmell
National Technical Information Service, Springfield, Virginia, 1983), CONF-820131, pp. 222-255

Proceedings of the Conference on Lasers in Nuclear Physics, Oak Ridge, Tennessee, 21-23 April 1982

On-Line Laser Spectroscopy with a Cooled He-Jet Transport System
David Lewis (Iowa State U.), Rollin Evans (Iowa State), Cary Davids, Miles Finn (U. Minnesota), George Greenlees (Minneosta), and Stanley Kaufman (Minnesota)
Ed. by C. E. Bemis, Jr. and H. K. Carter (Harwood Academic Publishers, NY, 1982), pp. 189-196

APS Meeting, Washington, D.C., 26-29 April 1982

Elastic Scattering and Reactions of ^{40}Ca + ^{40}CXa
R. R. Betts (CHM Div., ANL), I. Ahmad (CHM), B. B. Back (CHM), B. G. Glagola (CHM), W. Henning, S. Saini (CHM), and J. L. Yntema
Bull. Am. Phys. Soc. 27, 474 (1982)

Fusion, Fission and Deep-Inelastic Reaction Cross Sections for ^{32}S + ^{112,116,120,124}Sn
H. Ernst, C. N. Davids, W. S. Freeman, W. Henning, T. Humanic, F. W. Prosser (U. Kansas), and R. Racca (Kansas)
Bull. Am. Phys. Soc. 27, 475 (1982)

Measurement of the Beta Decay of ^{16}N(0$^-$, 120 keV): The Need for Meson Exchange Currents and the Value of g_P
C. A. Gagliardi, G. T. Garvey, S. J. Freedman (Stanford), and J. R. Wrobel
Bull. Am. Phys. Soc. 27, 492 (1982)

Fundamental Aspects of Nuclear Beta Decay
G. T. Garvey
Bull. Am. Phys. Soc. 27, 463 (1982)

APS, Washington, D.C., 26-29 April 1982 (contd.)

Search for Transient Electric Field Gradients Acting on Fast-Moving Ions in Solids
T. J. Humanic, H. Ernst, W. Henning, T. L. Khoo, Steven C. Pieper, and J. P. Schiffer
Bull. Am. Phys. Soc. 27, 520 (1982)

TOF Measurements of Evaporation Residues Produced in $^{16}O + ^{12}C$ and $^{16}O + ^{24}Mg$ at $4 \lesssim 9.4$ MeV/A
T. Humanic, D. G. Kovar, R. Betts (CHM Div., ANL), P. Chowdhury, D. Henderson, R. V. F. Janssens, W. Kühn, and K. Wolf (CHM)
Bull. Am. Phys. Soc. 27, 478 (1982)

Angular Momentum Dependence of Neutron Spectra in the 250-MeV $^{64}Ni + ^{92}Zr$ Reaction
W. Kühn, I. Ahmad (CHM Div., ANL), P. Chowdhury, R. V. F. Janssens, T. L. Khoo, F. Haas (Mich. State U.), J. Kasagi (MSU), and R. M. Ronningen (MSU)
Bull. Am. Phys. Soc. 27, 475 (1982)

Energy Dependence of $^{24}Mg + ^{24}Mg$ Elastic Scattering and Reactions
S. Saini (CHM Div., ANL), R. R. Betts (CHM), I. Ahmad (CHM), B. B. Back (CHM), G. B. Glagola (CHM), J. L. Yntema, R. W. Zurmuhle (U. Penn.), and F. Haas (Mich. State U.)
Bull. Am. Phys. Soc. 27, 480 (1982)

Measurement of the $^{2}H(\gamma,n)^{1}H$ Relative Cross Section at $E_\gamma \lesssim 19$ MeV
K. Stephenson, R. E. Holland, R. J. Holt, H. E. Jackson, R. D. McKeown, and J. R. Specht
Bull. Am. Phys. Soc. 27, 570 (1982)

High Intensity Inverted Sputter Source
J. L. Yntema and P. J. Billquist
Bull. Am. Phys. Soc. 27, 521 (1982)

30th Annual Conference on Mass Spectrometry and Allied Topics, Honolulu, Hawaii, 6-11 June 1982

Photoionization Mass Spectrometry of CH_3SH, CD_3SH and CH_3SD: Heats of Formation of $CH_3S^+(CH_2SH^+)$, CH_2S^+, CH_2S and HCS^+
R. E. Kutina, A. K. Edwards, G. L. Goodman, and J. Berkowitz
Proc. ed. by F. W. Lampe (American Soc. for Mass Spectrometry, 1982), Abstracts, pp. 617-618

Photoionization Mass Spectrometry of NH_2OH: Heats of Formation of HNO^+ and NOH^+
R. E. Kutina, G. L. Goodman, and J. Berkowitz
Proc. ed. by F. W. Lampe (American Soc. for Mass Spectrometry, 1982), Abstracts, pp. 504-505

30th Annual Conference on Mass Spectrometry and Allied Topics, Honolulu, Hawaii, 6-11 June 1982 (contd.)

Photoelectron Spectra of Gas Phase Lanthanide Trihalides
B. M. Ruscic, G. L. Goodman, and J. Berkowitz
Proc. ed. by F. W. Lampe (American Soc. for Mass Spectrometry, 1982), Abstracts, pp. 700-701

Proceedings of the 1982 INS International Symposium on Dynamics of Nuclear Collective Motion--High Spin States and Transitional Nuclei, Tokyo, Japan, 6-10 July 1982

Shell Structure at High Spin and the Influence on Nuclear Shapes
T. L. Khoo, P. Chowdhury, I. Ahmad (CHM Div., ANL), J. Borggreen, H. Emling, D. Frekers, R. V. F. Janssens, A. Pakkanen (Purdue U.), Y. H. Chung (Purdue), P. J. Daly (Purdue), S. R. Faber (Purdue), Z. Grabowski (Purdue), H. Helppi (Purdue), M. Kortelahti (Purdue), and J. Wilson (Purdue)
Ed. by K. Ogawa and K. Tanabe (Inst. for Nucl. Study, U. of Tokyo, Japan, Sept. 1982), pp. 256-274

International Conference on X-Ray and Atomic Inner-Shell Physics, Eugene, Oregon, 23-27 August 1982

The Effect of Inner-Shell Vacancies on Multiple Scattering Distributions of Heavy-Ion Beams Traversing Solids
E. P. Kanter
Ed. by B. Crasemann (U. of Oregon, 1982) Program and Abstracts, Vol. 1, pp. 132-133

Equilibration Lengths for K-Shell Charge-Exchange Processes for Fast Ions Traversing Foils - Evidence from Multiple-Scattering Distributions and Auger-Yield Measurements
Elliot P. Kanter, Dieter Schneider, and Donald S. Gemmell
Ed. by B. Crasemann (American Inst. of Physics, NY, 1982) pp. 735-744
+ Program and Abstracts (U. of Oregon, 1982), Vol 1, p. 169

Auger-Electron Spectroscopy on Foil and Gas Excited Fast-Atomic and Molecular-Ion Beams
D. Schneider, E. P. Kanter, D. S. Gemmell, and B. J. Zabransky
Ed. by B. Crasemann (U. of Oregon, 1982)
Program and Abstracts, Vol. 2, pp. 186-187

SNEAP '82 (Symposium of Northeastern Accelerator Personnel, Seattle, Washington, 6-8 Oct. 1982)

1982 SNEAP Tandem-Linac Accelerator Report
P. Den Hartog, R. Pardo, F. Munson, and C. Heath
Ed. by W. G. Weitkamp (Univ. of Washington, 1982), pp. 166-168

2.3 High Voltage Electron Microscope Tandem Facility

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

   Answer: The Electron Microscopy Center for Materials Research presently includes the High-Voltage Electron Microscope (HVEM) - Tandem Facility, two conventional transmission electron microscopes with analytical capabilities, and the developing state-of-the-art Analytical Electron Microscope. A wide variety of new materials science is being explored by researchers through particular capabilities offered in the HVEM-Tandem Facility of the Center. The large sample penetration offered by the high-energy electrons in the HVEM, for example, is enabling user scientists to investigate grain boundary structures and energies in high-temperature ceramics and new composite materials. In addition, the in situ observation of phase transformations, deformation, and fracture mechanisms in a variety of metallic and nonmetallic materials is being carried out at the Facility, owing to the available combination of thick-sample penetration and dynamic image-recording systems. Through the unique coupling of ion accelerators to the HVEM available in the HVEM-Tandem Facility, a wide variety of radiation-effects studies are being carried out for the first time. These include fundamental studies of defect formation in materials under ion irradiation, investigations of the redistribution of alloying elements and alloy phase stability in materials under electron and ion irradiation, direct observations of the ability to modify the microstructure and properties of materials by means of ion irradiation, and examination of the stability of nuclear-waste storage materials. Beyond these investigations, all being carried out in vacuo, the capability available in the HVEM-Tandem Facility for also studying materials under gaseous environments is enabling user researchers to study in situ for the first time the effects of hydrogen on the mechanical deformation and fracture characteristics of technologically important materials. The analytical electron microscopy capabilities in materials research are being expanded through fundamental studies of electron-solid interactions and the development of a high-spatial-resolution, ultra-high vacuum Analytical Electron Microscope which will advance the state-of-the-art in this area. In addition, the techniques of electron energy loss spectroscopy and x-ray energy dispersive spectroscopy are being applied to studies of radiation-induced solute segregation, oxidation of alloys, grain-boundary segregation and phase identification in steels, catalysis, superconductivity, and layered-ultrathin-coherent structures.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

   Answer: This Center for collaborative materials research allows unique combinations of experiments to be performed using the high-voltage electron microscope, a Kratos 1.2 MeV instrument, which is coupled via an instrumented beam line to two ion accelerators. The particular utility and uniqueness of the HVEM-Tandem Facility of the Center arises from the fact that microscope specimens can be bombarded in situ by beams of charged ions in a manner unavailable elsewhere in the world. The two alternative ion sources are, first, a National Electrostatics 2 MV Tandem Ion Accelerator and, second, a 300 kV, high current ion accelerator made by Texas Nuclear and equipped with sources for gaseous and metallic ions. The capability for ion damage using the available ion-beam instrumentation can be uniquely employed to simulate the damage caused by neutrons in a reactor environment or to investigate directly the damage that is introduced in ion implantation processes. The advanced Analytical Electron Microscope, which is currently being developed within the Center, will add to the unique features of the Center by making possible analytical investigations under ultra-high vacuum conditions, which will define the state-of-the-art in spatial resolution.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

Answer: The Center is currently comprised of a High-Voltage Electron Microscope (HVEM)-Tandem Accelerator Facility, which is a unique national users facility, and two more conventional electron microscopes. The HVEM, a Kratos 1.2 MeV model EM7, incorporates all recent design improvements and is equipped with a variety of side-entry specimen rods that permit observations from 10 to 1000 K in vacuo, and ambient to 1300 K in gaseous environments. Because foils ranging in thickness from 1 to 5 microns may be examined in the microscope, transformation and deformation processes can be examined in real-time in-situ experiments at temperatures of up to about half the foil melting temperature with significantly less interference from surface-dominated reactions than is encountered in conventional low-energy microscopy. Furthermore, the unique ion-beam interface system enhances the scope of the in-situ work by allowing change of the sample chemistry or structure through implantation or bombardment with a characterized beam of ions with energies between 10 keV and 8 MeV. Ion beams of most stable isotopes in the periodic table can be made available from the 300-kV Texas Nuclear Accelerator and the 2-MV National Electrostatics, Inc. Tandem Accelerator situated in the accelerator facility adjacent to the HVEM and connected to it via a fully instrumented beam line. Real-time changes in microstructure can be video recorded; a video editing system is also available. The more conventional electron microscopes in the Center are a JEOL 100 CX transmission and scanning transmission electron microscope (TEM/STEM) with an X-ray energy dispersive spectrometmer (XEDS) and a Philips EM 400 equipped with XEDS and an electron energy loss spectrometer (EELS). A new generation, medium voltage, high spatial resolution, ultra-high vacuum Analytical Electron Microscope, with substantially increased capabilities over the present-day instruments is in the process of being acquired by the Center.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer: A number of exciting research projects have been carried out within the Electron Microscopy Center for Materials Research since FY 1981. These have included investigations using the variety of special capabilities of the HVEM-Tandem Facility as well as those of the analytical electron microscopes available within the Center. Only a few highlights from this large body of research can be cited here.

Displacement cascade collapse in Cu_3Au has been successfully studied at low temperatures (below 30 K) in the liquid-He stage of the HVEM-Tandem Facility by T. J. Black and M. L. Jenkins (University of Oxford, U.K.) and M. A. Kirk (ANL). Thin foil samples were irradiated in situ with Ar^+, Cu^+ and Kr^+ ions, ranging in energy from 50 to 100 keV, up to a dose of about 2×10^{15} ions m^{-2}. The HVEM was operated at 300 kV, below the threshold for electron irradiation damage in Cu_3Au. The results confirm that, under the experimental conditions used, cascade collapse does occur at irradiation temperatures down to T = 10 K, and shed light on the important but poorly understood mechanism by which the vacancy-rich cores of displacement cascades collapse to dislocation loops in irradiated metals and alloys (1982).

Measurements of the growth rate of segregation-induced Ni_3Si surface films on Ni-Si alloys during electron irradiation in the HVEM have provided an important step toward correlating elevated temperature radiation effects produced by electrons and charged particle irradiations. By exploiting the dose-rate dependence of the film growth rates derived from previous theoretical studies and ion irradiation experiments, T. Muroga, P. R. Okamoto and H. Wiedersich (ANL) have obtained estimates of the defect production efficiencies of 1 MeV electrons. Defect production efficiency is defined as the fraction of defects that is free to migrate and contribute to microstructural changes. The results imply that 1 MeV electrons are about 1.5 fold as efficient as 1 MeV H^+ ions, or that the formula normally used to calculate the atomic displacement rate for 1 MeV electrons underestimates the displacement cross-section by about 50% (1982).

A study of defect clustering during electron irradiation of Pt-C alloys by P. Regnier, visiting scientist from CEN-Saclay, N. Q. Lam, ANL, and K. H. Westmacott, Lawrence Berkeley Laboratory, has provided new insight into the mechanisms of microstructural changes in interstitial alloys during irradiation at energies below the displacement threshold of the matrix atoms. The observed microstructures showed the growth of black dots within the carbon precipitates and in the precipitate-free matrix. At higher doses the black dots multiply and grow into dislocations loops. The formation of these interstitial dislocation loops indicates that platinum atoms are displaced by secondary C-Pt collisions. This work indicates the importance of accounting for secondary-collision processes in the assessment of irradiation damage in alloys having drastically different atomic masses.

T. Schober, visiting scientist from KFA, Julich, working with M. Chason, ANL, completed a CTEM and HVEM study of hydride precipitation in magnesium - an important candidate for reversible storage of hydrogen. Samples were studied at temperatures of < 170 K to avoid radiolytic decomposition of the samples. The orientation relationships between the hydrides and the matrix were established in hydrogen loaded samples and the production of small random Mg grains during dehydration was also observed (1983).

The damage function, the average number of Frenkel pairs created as a function of lattice atom recoil energy, was investigated in Cu and Ni using in-situ electrical-resistivity damage-rate measurements in the HVEM at T < 10 K. The research was carried out by W. E. King, and K. L. Merkle from ANL and A. C. Baily. K. Haga, and M. Meshii from Northwestern University. Electron and proton irradiations were performed in-situ on the same polycrystalline specimens using the HVEM-Ion Beam Interface. Both Ni and Cu exhibit a sharp rise in the damage function above the minimum threshold energy (~18 eV for Cu and ~ 20 eV for Ni) as displacements in the low threshold energy regions of the threshold energy surface become possible. A plateau is observed for both materials (0.54 Frenkel pairs for Cu and 0.46 Frenkel pairs of Ni) indicating that no further directions become productive until much higher recoil energies. These damage functions show strong deviations from simple theoretical models, such as the Modified Kinchin-Pease damage function (1983).

It has been known for over 40 years that trace (< 1% by weight) additions of reactive elements like Y, Ce, and Hf, or oxide dispersions of these elements in Cr-bearing alloys result in reduction in the growth rate of the oxide scales and enhancement in scale adhesion under high-temperature isothermal and cyclic oxidation conditions. However, conventional kinetics studies and metallographic examinations have not led to the mechanism for this so-called "reactive-element" effect. Analytical electron microscopy has been used by W. E. King, N. L. Peterson and J. F. Reddy, ANL, to investigate the microstructure and elemental distributions in oxide scale, at the metal:oxide interface, and in the base metal for three alloys, Fe-24Cr, Fe-24Cr-0.07Y, and Fe-24Cr-0.87Y. Samples were oxidized at 1000°C for various times in pure oxygen. Oxidized samples were transverse sectioned and prepared for electron optical observation and microanalysis. The results indicate that the origin of the "reactive-element" effect is to be found in the base alloy, not in the scale as has been proposed by previous investigators (1984-1985).

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

   Answer: Within the HVEM-Tandem Facility of the Center, the interface between the HVEM and the accelerators was established and instrumented, and the 2-MV ion accelerator was converted to tandem operation, during FY 81-82. At present, a double-tilt liquid-He cooled specimen stage is being fabricated for the HVEM; it will be available for use in the Center toward the end of FY 1984. In addition, the HVEM vacuum system has been improved to allow for investigations of materials sensitive to residual-gas impurities over a wider range of temperatures, and a video image-recording system was installed to allow for in situ recording of dynamic studies. In order to increase the scientific capabilities of the Center, sample analytical probes are being designed and installed in the HVEM. These include systems for electron-energy-loss spectroscopy (EELS) and x-ray energy-dispersive spectroscopy (XEDS). A microfocus capability for the ion-beam interface is also planned to enable in situ ion-beam analysis techniques to be used in the HVEM by the end of FY 1985. These analytical probes have been designed based on research and developments in analytical electron microscopy (EELS and XEDS) carried out on the Center's more conventional electron microscopes. The Phillips EM 400 was purchased prior to FY 1981, but during the subsequent period was modified for both EELS and XEDS capabilities. The JEOL 100 CX was purchased in FY 1982 in replacement of an earlier version of this microscope. An advanced medium-voltage, high spatial resolution, ultra-high vacuum Analytical Electron Microscope is now in the process of being procured for delivery in FY 1986.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer: Electron Microscopy Center for Materials Research Budget Profile
(B/A in thousands of $)

	FY 1981	FY 1982	FY 1983	FY 1984*	FY 1985*	Source of Funds
Facility Operation	560	550	615	685	750+	Materials Sciences
User Interfacing (1)	10	10	15	20	25	
In-house Research	600	750	970	1,280	1,460	Materials Sciences
User Research Support (2)	500	650	750	800	1,200+	
Capital Equipment	370	35	235	900	925	Materials Sciences
GPP	0	0	0	200	800	

(1) Scientific assistance is provided through the in-house research program. These funds are used for travel and living expenses for users requiring same, and are provided by The University of Chicago.

(2) These totals represent our estimates of the research support provided non-Argonne facility users through their home institutions for work in which the Argonne facility plays a prominent role.

* Estimated

+ Assuming the operation schedule is extended beyond 40 hrs/week.

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer: None.

8. **For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.**

Answer: Both total direct staffing (operations) of the Center and the use by Argonne research staff are shown.

	FY 1981	FY 1982	FY 1983	FY 1984*	FY 1985*
Total direct staffing (FTE)	4.4	4.4	6.3	6.0	8.0
In-house research staffing (FTE)	13.5	14.0	13.5	14.0	18.0

* Estimated

9. What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?

Answer: The utilization of the Center for the period FY 1981 - FY 1985 is shown below. Full utilization of the Center is based upon five 8-hour shifts (i.e., a 40-hour week)

	FY 1981	FY 1982	FY 1983	FY 1984*	FY 1985*
Actual use in 8-hour shifts	269	304	258	300	312
Full use in 8-hour shifts	245	259	217	240	240
% of full use (40-hour week)	110%	117%	119%	125%	130%

* Estimated

Complete utilization of this facility would involve about 640 shifts/year.

10. For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?

Answer: The number of experiments in the Center which have been started, continued, and completed during the period FY 1981 - FY 1985 are as follows:

	FY 1981	FY 1982	FY 1983	FY 1984*	FY 1985*
Started	17	22	20	24	28
Continued	18	14	20	22	23
Completed	16	16	15	21	23
Publications	19	52	28	38	45

* Estimated

11. What is this facility's user policy?

Answer: The Electron Microscopy Center for Materials Research has a well-defined user policy for the HVEM-Tandem Facility, which is the only national users facility currently available within the Center. (An appropriate user policy for the new advanced Analytical Electron Microscope will be developed within the next year in conjunction with the HVEM-Tandem Facility Steering Committee.) The user policy for the HVEM-Tandem Facility has been established by the management of the Materials Science and Technology (MST) Division at ANL with advice from a HVEM-Tandem Facility Steering Committee made up of eight representatives from academic and industrial research institutions and seven ANL/MST research staff members. The chairperson of the Committee is elected annually by the members. The Steering Committee handles general matters of Facility development and evaluation of research proposals and use priorities for the Facility. Priority use of the Facility is for fundamental materials research that will be published in the open literature. All major use of the

HVEM-Tandem Facility is obtained through research or technical proposals submitted to the Steering Committee. The criteria for evaluation of a proposal and the allotment of use time include scientific merit, feasibility, need for the use of these unique facilities, and compatibility of the proposed research with Facility equipment and operational priorities. In general, the Committee seeks to maintain an approximately 50% non-ANL usage of schedulable time. All users with approved research proposals have priority use of Facility equipment. Requests for minor use of the Facility may be discussed directly with the Facility manager. The provision for limited usage is intended to provide time for exploratory investigations.

Scientists from universities and government and industrial laboratories are invited to use the Electron Microscopy Center for Materials Research and its HVEM-Tandem Facility in furthering their research. However, any activity which can be carried out through commercially available laboratories, such as that which can be performed on the Center's more conventional microscopes, is not appropriate for this Center.

While there are no use charges for basic research, the users are responsible for all expenses associated with their research. Facility funds permit replacement of malfunctioning equipment subjected to normal use, but the cost of replacement of items damaged by a user because of negligent or improper operation may be levied against the research funds. Industrial users wishing to carry out proprietary research are charged for the use of the Facility.

Users must give credit to the sponsoring agency (DOE/BES) of the Facility in all reports, publications and presentations arising from use of the Facility. Facility staff are available during one or two shifts a day to instruct experimenters in the use of the equipment, and in some instances to participate in experimental programs. Since Facility staff must maintain and upgrade the facility equipment, it is expected that researchers will become competent to operate the equipment without ANL assistance. To this end, a course of lectures on high-voltage electron microscopy has been given and is available on videotape together with supplemental lecture notes for potential users. Research proposals are normally accepted for eighteen months of work, but may be renewed. Sixteen months after the acceptance of a proposal, the authors should submit a report summarizing their work, together with copies of other reports and publications and a list of oral presentations. Proposals for modifications of the Facility systems must be submitted to the Steering Committee for approval and then scheduled by the manager. Equipment that is developed for use with the Facility through these projects shall in general become the property of the Facility after the first anniversary of its initial use. The user shall provide the Facility staff with adequate documentation to allow service and use of the equipment by other workers.

12. For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?

Answer: During the period FY 1981 to the present no reimbursable research has taken place at the Facility. It is anticipated that very limited reimbursable research will take place at the Facility through FY 1985. Such research planned by Shell Oil Co. should amount to about $2000 (i.e., 16 hours at $125 per hour) during the remainder of FY 1984. A similar amount within a factor of three might be anticipated for FY 1985.

13. **What is the mechanism by which specific research proposals for experiments at the facility are considered?**

Answer: A proposal for use of the HVEM-Tandem Facility within the Center should be submitted to the Facility manager at least one month before a scheduled meeting of the Steering Committee to provide the Committee with sufficient time to evaluate the proposal. A proposal shall consist of a completed proposal summary sheet, and two typewritten pages with the following format and content:

i. Title of Proposal and Authors
ii. Scientific Objective of Proposed Research
iii. Justification of Need to Use HVEM-Tandem Facility
iv. Short Description of Method and Equipment Requirements
v. List of Materials to be Examined and Possible Contamination Problems, e.g., High Vapor Pressures, Corrosion, Spallation, and Corrosive Activity

Proposals are reviewed by two key readers appointed by the chairperson of the Steering Committee; they may be either Committee members or outside experts in the appropriate field. The decision, which is by open ballot recorded in the minutes, is communicated to the authors by the Facility manager, who serves as the Committee secretary. All users with approved research proposals have priority use of Facility equipment. An appropriate proposal mechanism for use of the advanced Analytical Electron Microscope will be developed prior to its availability for research.

14. **How many research proposals have been submitted over the past five years, and how many of these have been approved?**

Answer: During the past five years, 125 research proposals have been submitted for use of the HVEM-Tandem Facility, the only facility of the Electron Microscopy Center for Materials Research presently requiring such proposals. Approximately 90% of these (112) have been approved. However, many of the proposals are revised or the requested amount of use time reduced at the behest of the Steering Committee. This accounts for the relatively large percentage of acceptance.

15. **How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?**

Answer: Over the past five years, 150 university personnel, including faculty and students, have utilized the HVEM-Tandem Facility of the Center.

16. How many industrial researchers have utilized the facility over the past five years?

Answer: Over the past five years, 10 industrial researchers have utilized the HVEM-Tandem Facility of the Center.

17. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer: Over the past five years, 6 researchers from foreign institutions have utilized the HVEM-Tandem Facility of the Center.

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: None. ("Researchers from other agencies" are defined as regular full-time employees of agencies, federal or state, other than DOE or GOCO contractors.) It should be noted that scientists from other DOE laboratories do use the facility.

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: The cornerstone of the Electron Microscopy Center for Materials Research at Argonne is the existing HVEM-Tandem Facility, which is already a world-class, unique facility for the investigation of materials in a high-voltage electron microscope (HVEM) under realistic conditions within a variety of gaseous and irradiation environments. The capabilities of the HVEM-Tandem Facility can be considerably expanded by the addition of an electron energy-loss spectrometer to the HVEM and the improvement of low-temperature capabilities through design and construction of a double-tilt He-cooled specimen stage. Both of these projects are now in progress and are being funded within the limits of normal operating and equipment budgets.

20. Please provide a copy of the facility's latest annual report.

Answer: The Electron Microscopy Center for Materials Research does not at present publish an annual report. In lieu of this, the HVEM-Tandem Facility does contribute on a regular basis to a semi-annual Newsletter, put together at ANL under the auspices of the Facility and DOE/BES Division of Materials Sciences (DMS), which reports on the various high-voltage electron microscopy efforts supported by the DOE/BES-DMS program, including those in the BES-supported Electron Microscopy Centers at ANL and LBL. A copy of the most recent Newsletter is attached, as is a copy of the Facility's section from the most recent Annual Report of the Materials Science and Technology Division at Argonne.

HVEM-TANDEM FACILITY

A. Taylor, Facility Manager

A. Philippides
S. L. Ruffatto
(Secretary)*
E. A. Ryan
J. R. Wallace

Introduction

The ANL-Materials Science and Technology Division High Voltage Electron Microscope (HVEM)-Tandem Facility is a unique national research facility available without charge to scientists from industry, universities, and other national laboratories, following a peer evaluation of their research proposals by the Facility Steering Committee. Through critical review of proposals, the steering committee, in collaboration with MST management, endeavors to encourage full exploitation of the facility's unique capabilities for high-quality, publishable materials research in support of various energy technologies. A guideline has been established whereby prime-time usage of the facility is divided approximately equally between ANL and non-ANL scientists.

The HVEM, a Kratos model EM7, incorporates all recent design improvements and is equipped with a variety of side-entry specimen rods that permit observations from 10 to 1000 K in vacuo, and ambient to 1300 K in gaseous environments. Because foils ranging in thickness from 1 to 5 μm may be examined in the microscope, transformation and deformation processes can be examined in real-time in-situ experiments at temperatures of up to about half the foil melting temperature with significantly less interference from surface-dominated reactions than is encountered in conventional low-energy microscopy. Furthermore, the unique ion beam interface system enhances the scope of the in-situ work by allowing change of the sample chemistry or structure through implantation or bombardment with a characterized beam of ions with energies between 10 keV and 8 MeV. Ion beams of most stable isotopes in the periodic table can be made available from the 300-kV Texas Nuclear Accelerator and the 2-MV National Electrostatics, Inc. Tandem Accelerator situated in the accelerator facility adjacent to the microscope. Real-time changes in microstructure can be video recorded. A video editing system is also available.

The accelerator facility, which may be operated independently of the microscope, has provision for five beam-line locations three of which are, or will shortly be, in use. The 30°E target chamber is set up for implantation and routine sample analysis using nuclear reactions and Rutherford backscattering techniques. A Nuclear Data ND6600 system is available for on-line data acquisition and analysis. The 10°E target chamber is being set up to accept ion beams from both accelerators (dual-beam system) so as to provide simultaneous monitoring of implantation processes as well as dual-ion irradiations. The target chamber on the 20°E beam line is equipped for ion implantation of large specimens.

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*Serves two groups.

Members of the facility staff provide system maintenance and train users to operate the equipment. In general, users are encouraged either to provide sufficient manpower to carry out their own experiments, or to collaborate with MST staff. The availability of the facility has been widely publicized through news releases, journal publications, and presentations at meetings of professional societies. A bulletin is issued periodically to keep users informed of recent work at the facility and of system improvements. Sixteen hours of videotaped lectures from Part I of the HVEM 1982 Summer Institute are available for prospective users. To date, 18 groups have participated in the two-day training session which constitutes Part II of the Institute.

Facility Development

Major improvements and additions to the facility have been recommended by the steering committee and are proceeding as facility work projects. Current projects include (1) design and installation of an electron-loss spectrometer in collaboration with N. Zaluzec (Kinetics and Ion Irradiation Group) and (2) design and construction of a double-tilt He-cooled stage in collaboration with A. Baily and K. Haga (Northwestern University) and W. King and K. L. Merkle (Defects in Ceramics Group).

A new skim-cup and moveable Faraday cup were installed inside the microscope to define and characterize the ion beam.

Results

Table I summarizes the research carried out at the HVEM from 1981 to the present. Throughout FY 1983, emphasis has been placed on training users, carrying out experiments, and gaining operational experience with the Tandem Accelerator. During this period, the HVEM has provided reliable service, on a six days/week schedule, for some 28 research groups with programs approved by the Steering Committee. About 65% of the schedule has been assigned to university and industrial users; approximately half of the outside use involves research in collaboration with MST staff. In terms of the types of projects carried out, the use of the HVEM during FY 1983 encompassed four general areas: studies of large-scale structure (11 projects), mechanical behavior (3 projects), solute segregation effects (2 projects), and radiation damage (12 projects). Nine projects involved use of the microscope and the ion beam interface to study various ion beam effects. Considerable experience has been gained in carrying out ion beam irradiations at 10 K and in imaging the resultant damage cascades at low temperatures.

The Tandem Accelerator is now used by the Kinetics and Ion Irradiation Group on a regular basis for ion irradiation and RBS work. Three programs of applied research with the Tandem Accelerator have been initiated by G. Fenske (Ceramics Group, Materials Technology) in collaboration with outside users.

TABLE I. INVESTIGATIONS CARRIED OUT BY HVEM USERS FROM 1981 TO THE PRESENT

TOPIC	USER	AFFILIATION
	STRUCTURE STUDIES (LARGE-SCALE DEFECTS)	
Si/SiO_2 INTERFACES	PINNIZZOTTO, VAANDRAGER	TEXAS INSTRUMENTS
TUNGSTEN BRONZES	KRAUSE	NORTHERN ILLNOIS UNIV.
DISLOCATION STRUCTURE IN UO_{2+x}	HEUER, KELLER	CASE WESTERN RESERVE UNIV.
ZIRCALOY CLADDING	CHUNG	ANL
SINTERING OF ALUMINA	PHILLIPS	UNIV. OF ILLINOIS
MICROSTRUCTURE OF DICALCIUM SILICATE	YOUNG, GHOSE, CHOPRA	UNIV OF ILLINOIS, ANL
VOIDS INDUCED BY CREEP & FATIGUE	WEERTMAN, KIM, YANG	NORTHWESTERN UNIV.
GRAIN BOUNDARY ENERGIES IN Au	CHAN, BALLUFFI	MIT
SILICATES IN SANDSTONE	HURD, SEARS	SHELL OIL
C-FLUID PRECIPITATION IN OLIVINES	GREEN, VAUGHAN	UNIV. OF CALIF.-DAVIS
	IN-SITU MECHANICAL DEFORMATION (STRAINING OF FOILS)	
EFFECT OF H_2 ON FRACTURE	BIRNBAUM, ROBERTSON, TOBATA	UNIV. OF ILLINOIS
STRUCTURE AND FRACTURE PROPAGATION	RIGSBEE	UNIV. OF ILLINOIS
NEUTRON IRRADIATION EFFECTS	LOOMIS, GERBER	ANL
DEFORMATION IN SPINODAL ALLOYS	SUBRAMANIAN	MICH. STATE UNIV.

Table I (Contd.)

TOPIC	USER	AFFILIATION
IN-SITU IRRADIATION DAMAGE (ε^- AND IONS)		
DEFECT PRODUCTION IN PURE METALS	BAILY, HAGA, MESHII	NORTHWESTERN UNIV.
CASCADES IN Fe	ROBERTSON, KIRK	UNIV. OF ILLINOIS, ANL
CASCADES IN ORDERED ALLOYS	JENKINS, BLACK, KIRK	UNIV. OF OXFORD, ANL
VOID FORMATION IN ALLOYS	STUBBINS	UNIV. OF ILLINOIS
DAMAGE IN NUCLEAR WASTE GLASSES	DeNATALE, HOWITT, MITCHELL	UNIV. OF CALIF.-DAVIS
DAMAGE IN OXIDES	CARTZ, KARIORIS, FOURNELLE	MARQUETTE UNIV.
DEFECT PRODUCTION EFFICIENCIES AT HIGH TEMPERATURE	MUROGA, OKAMOTO, REHN	UNIV. OF TOKYO, ANL
IN-SITU SOLUTE-DEFECT INTERACTIONS (ε^- AND IONS)		
CARBIDE INSTABILITY IN Ni	REGNIER, LAM, WESTMACOTT	SACLAY, ANL, LBL
SURFACE SEGREGATION IN Ni-Si	WAGNER, REHN, AVERBACK	ANL
SEGREGATION IN Mo-Rh	ERCK, WIEDERSICH	ANL
PHASE TRANSITIONS IN CRISTOBALITE	HEUER, NORD	CASE WESTERN RESERVE UNIV.
INTERMETALLIC FORMATION IN THIN FILMS	ALLEN, WIEDERSICH	NOTRE DAME, ANL
OTHER		
HVEM-EELS	ZALUZEC, FACILITY STAFF	ANL

HVEM-Tandem Facility: Publications by MST Staff
(October 1, 1982 to June 30, 1983)

Papers

THERMOMECHANICAL ASPECTS OF FUEL-ROD MATERIAL INTERACTIONS AT $\lesssim$1900°C. H. M. Chung and S. M. Gehl (Electric Power Research Institute, Palo Alto, CA). Proc. of the Intl. Mtg. on Thermal Nuclear Reactor Safety, Chicago, IL, August 29-September 2, 1982, NUREG/CP-0027, Vol. 2, February 1983, pp. 938-950

MOLECULAR DYNAMICS SIMULATION OF DISPLACEMENT CASCADES IN Cu: ANALYSIS OF REPLACEMENT SEQUENCES. Wayne E. King and R. Benedek. Point Defects and Defect Interactions in Metals, ed. Jin-ichi Takamura, Masao Doyama, and Michio Kiritani (Proc. Yamada Conf. V, Kyoto, Japan, November 16-20, 1981), Yamada Science Foundation, University of Tokyo Press, Tokyo, Japan, 1982, pp. 807-810

RE-EXAMINATION OF THE THRESHOLD ENERGY SURFACE IN COPPER. Wayne E. King, R. Benedek, K. L. Merkle, and M. Meshii (Northwestern University, Evanston, IL). INVITED PAPER. Point Defects and Defect Interactions in Metals, ed. Jin-ichi Takamura, Masao Doyama, and Michio Kiritani (Proc. Yamada Conf. V, Kyoto, Japan, November 16-20, 1981), Yamada Science Foundation, University of Toyko Press, Tokyo, Japan, 1982, pp. 789-794

STUDIES OF DEFECT PRODUCTION BY HIGH VOLTAGE ELECTRON MICROSCOPY AND IN-SITU ELECTRICAL RESISTIVITY. Wayne E. King, K. L. Merkle, and M. Meshii (Northwestern University, Evanston, IL). Advanced Techniques for Characterizing Microstructures, ed. F. W. Wiffen and J. A. Spitznagel (Proc. 109th AIME Ann. Mtg., Las Vegas, NV, February 26-28, 1980), The Metallurgical Society of AIME, Warrendale, PA, 1982, pp. 157-169

SURFACE SEGREGATION MEASUREMENTS DURING ELECTRON IRRADIATION. T. Muroga, P. R. Okamoto, and H. Wiedersich. Radiat. Eff. Lett. 68(6), 163-167 (February 1983)

MECHANISM AND KINETICS OF RADIATION-INDUCED SEGREGATION IN Ni-Si ALLOYS. P. R. Okamoto, L. E. Rehn, R. S. Averback, K.-H. Robrock (Institut für Festkörperforschung der Kernforschungsanlage, Jülich, W. Germany), and H. Wiedersich. Point Defects and Defect Interactions in Metals, ed. Jin-ichi Takamura, Masao Doyama, and Michio Kiritani (Proc. Yamada Conf. V, Kyoto, Japan, November 16-20, 1981), Yamada Science Foundation, University of Toyko Press, Tokyo, Japan, 1982, pp. 946-949

RADIATION-INDUCED MICROSTRUCTURAL CHANGES IN Ni-C AND Pt-C ALLOYS. P. G. Régnier (CEN, Saclay, France) and N. Q. Lam. Dimensional Stability and Mechanical Behaviour of Irradiated Metals and Alloys (Proc. Intl. Conf., Brighton, England, April 11-14, 1983), British Nuclear Energy Society, London, 1983, pp. 51-54

MICROSTRUCTURAL TRANSITIONS IN Pt-C ALLOYS DURING HIGH-VOLTAGE-ELECTRON-MICROSCOPE IRRADIATION. P. G. Régnier, N. Q. Lam, and K. H. Westmacott (Lawrence Berkeley Laboratory, Berkeley, CA). J. Nucl. Mater. 115(2&3), 286-296 (April 1983)

EFFECT OF DEFECT PRODUCTION RATE ON RADIATION-INDUCED SEGREGATION. L. E. Rehn, P. R. Okamoto, R. S. Averback, W. Wagner, and H. Wiedersich. Scr. Metall. 16(5), 639-642 (May 1982)

RECENT WORK USING THE ANL HVEM-ION BEAM INTERFACE. A. Taylor and E. A. Ryan. 1982 IEEE Conf. on the Application of Accelerators in Research and Industry, ed. J. L. Duggan and I. L. Morgan (Proc. Conf., North Texas State University, Denton, TX, November 8-10, 1982), IEEE Trans. Nucl. Sci. NS-30(2), April 1983, pp. 1263-1265

Abstracts and Summaries

TEM-HVEM OBSERVATION OF ORDERED ZIRCONIUM-OXYGEN PHASE IN ZIRCALOY SPENT-FUEL CLADDING. H. M. Chung. To be presented at Intl. Symp. on Environmental Degradation of Materials in Nuclear Power Systems - Water Reactors, Myrtle Beach, SC, August 22-24, 1983

THE COLLAPSE OF DEFECT CASCADES TO DISLOCATION LOOPS IN IRON AT 10 K. M. A. Kirk, I. M. Robertson, and W. E. King. To be presented at Seventh Intl. Conf. on High Voltage Electron Microscopy, Berkeley, CA, August 16-19, 1983

OBSERVATIONS OF IN-SITU TENSILE DEFORMATION AND FRACTURE IN NEUTRON-IRRADIATED NIOBIUM IN AN HVEM. B. A. Loomis and M. P. Otero (Inst. Pesqs. Energéticas e Nucleares, CNEN, Sao Paulo, Brasil). To be presented at 3rd Top. Mtg. on Fusion Reactor Materials, Albuquerque, NM, September 19-22, 1983

ANL HIGH VOLTAGE ELECTRON MICROSCOPE-TANDEM FACILITY. A. Taylor. Bull. Am. Phys. Soc. 28(3), Poster FX-1, p. 396 (March 1983) (Am. Phys. Soc. Mtg., Los Angeles, CA, March 21-25, 1983)

POTPOURRI AND PERSONALIA - HIGH-VOLTAGE ELECTRON MICROSCOPY COURSE. A. Taylor. NEWS ITEM. Bull. Electron Microscopy Society of America 12(2), 104-105 (July 1982)

RECENT WORK USING THE ANL-HVEM-ION BEAM INTERFACE. A. Taylor. Bull Am. Phys. Soc. 27(7), 791 (September 1982)

IN-SITU INVESTIGATION OF MATERIALS BEHAVIOR AT THE ANL HVEM-TANDEM FACILITY. A. Taylor and P. R. Okamoto. To be presented at TMS-AIME Fall Mtg., Philadelphia, PA, October 2-6, 1983

QUANTITATIVE ANALYSIS OF RADIATION-INDUCED SEGREGATION IN CONCENTRATED Ni-Cu ALLOYS. W. Wagner (Hahn-Meitner-Institut für Kernforschung, Berlin, W. Germany), V. Naundorf (Hahn-Meitner-Institut für Kernforschung, Berlin, W. Germany), L. E. Rehn, and H. Wiedersich. Presented at the Deutsche Physikalische Gesellschaft E. V. (German Physical Society), Freudenstadt, W. Germany, March 21-25, 1983

SURFACE-SEGREGATION OF THE ORDERED Ni_3Si PHASE DURING IRRADIATION. W. Wagner (Hahn-Meitner-Institut für Kernforschung, Berlin, W. Germany), L. E. Rehn, and H. Wiedersich. Verhandlungen DPG 5, 903 (1982)

Reports

ANALYSIS OF BRITTLE-TYPE FAILURE OF BIG ROCK POINT REACTOR FUEL CLADDING AFTER STRESS RUPTURE TESTING. H. M. Chung. Materials Science Division Light-Water-Reactor Safety Research Program: Quarterly Progress Report, April-June 1982, NUREG/CR-2970, Vol. II, ANL-82-41, Vol. II (May 1983), pp. 72-79

Submitted Papers

IN-SITU STUDIES OF CASCADE DEFECT FORMATION AT $T < 10$ K. K. Haga (Northwestern University, Evanston, IL), A. C. Baily (Northwestern University, Evanston, IL), Wayne E. King, K. L. Merkle, and M. Meshii (Northwestern University, Evanston, IL). To be published in Proc. Seventh Intl. Conf. on High Voltage Electron Microscopy, Berkeley, CA, August 16-19, 1983

MOLECULAR DYNAMICS SIMULATION OF LOW ENERGY DISPLACEMENT CASCADES IN Cu. Wayne E. King and R. Benedek. INVITED PAPER. Presented at TMS-AIME Fall Mtg., St. Louis, MO, October 24-28, 1982 (to be published in J. Nucl. Mater.)

IN-SITU OBSERVATION OF THE ENERGY DEPENDENCE OF DEFECT PRODUCTION IN Cu AND Ni. Wayne E. King, K. L. Merkle, A. C. Baily (Northwestern University, Evanston, IL), K. Haga (Northwestern University, Evanston, IL), and M. Meshii (Northwestern University, Evanston, IL). To be published in Proc. 7th Intl. Conf. on High Voltage Electron Microscopy, Lawrence Berkeley Laboratory, Berkeley, CA, August 16-19, 1983

THRESHOLD ENERGY SURFACE AND FRENKEL PAIR RESISTIVITY FOR Cu. Wayne E. King, K. L. Merkle, and M. Meshii (Northwestern University, Evanston, IL). Presented at TMS-AIME Fall Mtg., St. Louis, MO, October 24-28, 1982 (to be published in J. Nucl. Mater.)

VOID FORMATION AND SOLUTE SEGREGATION IN ION-IRRADIATED NIOBIUM-BASE ALLOYS. B. A. Loomis and S. B. Gerber. Presented at TMS-AIME Fall Mtg., St. Louis, MO, October 24-28, 1982 (to be published in J. Nucl. Mater.)

EXPERIMENTAL DETERMINATION OF THE ENERGY DEPENDENCE OF DEFECT PRODUCTION. K. L. Merkle, Wayne E. King, A. C. Baily (Northwestern University, Evanston, IL), K. Haga (Northwestern University, Evanston, IL), and M. Meshii (Northwestern University, Evanston, IL). Presented at TMS/AIME Fall Mtg., St. Louis, MO, October 24-28, 1982 (to be published in J. Nucl. Mater.)

SURFACE SEGREGATION IN CONCENTRATED Ni-Cu ALLOYS UNDER IRRADIATION. W. Wagner (Hahn-Meitner-Institut für Kernforschung Berlin, Berlin, W. Germany), V. Naundorf (Hahn-Meitner-Institut für Kernforschung Berlin, Berlin, W. Germany), L. E. Rehn, and H. Wiedersich. To be published in Proc. Eleventh Intl. Symp. on Effects of Radiation on Materials, Scottsdale, AZ, June 28-30, 1982

HIGH VOLTAGE ANALYTICAL ELECTRON MICROSCOPY. N. J. Zaluzec, A. Taylor, E. A. Ryan, and A. Philippides. To be published in Proc. Seventh Intl. Conf. on High Voltage Electron Microscopy, Berkeley, CA, August 16-19, 1983

HVEM-Tandem Facility: Publications by Other Users
(October 1, 1982 to June 30, 1983)

Papers

NATIONAL RESOURCES IN ELECTRON MICROSCOPY: THE MATERIALS SCIENCE DIVISION HVEM-TANDEM FACILITY AT ARGONNE NATIONAL LABORATORY. John J. Hren (University of Florida, Gainesville, FL). Bull. Electron Microscopy Society of America (EMSA) 13(1), 19-21, 24, and 26-27 (Spring 1983)

DEFECT AGGREGATION IN IRRADIATED Ni_3Al AND NiAl. H. C. Liu (Case Western Reserve University, Cleveland, OH) and T. E. Mitchell (Case Western Reserve University, Cleveland, OH). J. Nucl. Mater. 107, 318-326 (1982)

DEFECT STRUCTURES IN β-NiAl AND THEIR RESPONSE TO ELECTRON IRRADIATION. H. C. Liu (Case Western Reserve University, Cleveland, OH) and T. E. Mitchell (Case Western Reserve University, Cleveland, OH). Point Defects and Defect Interactions in Metals, ed. Jin-ichi Takamura, Masao Doyama, and Michio Kiritani (Proc. Yamada Conf. V, Kyoto, Japan, November 16-20, 1981), Yamada Science Foundation, University of Tokyo Press, Tokyo, Japan, 1982, pp. 635-638

A HVEM STUDY OF RADIATION-INDUCED SEGREGATION IN DILUTE Ni-Be ALLOYS. T. Mukai (Case Western Reserve University, Cleveland, OH) and T. E. Mitchell (Case Western Reserve University, Cleveland, OH). Point Defects and Defect Interactions in Metals, ed. Jin-ichi Takamura, Masao Doyama, and Michio Kiritani. (Proc. Yamada Conf. V, Kyoto, Japan, November 16-20, 1981), Yamada Science Foundation, University of Tokyo Press, Tokyo, Japan, 1982, pp. 950-953

NATURE OF DISLOCATION LOOPS IN ELECTRON-IRRADIATED CuAuI AND Cu_3Au. T. Mukai (Case Western Reserve University, Cleveland, OH) and T. E. Mitchell (Case Western Reserve University, Cleveland, OH). Phil. Mag. A 45(5), 741-751 (1982)

RADIATION-INDUCED HOMOGENEOUS PRECIPITATION IN Ni-1 at% Be ALLOYS. T. Mukai (Case Western Reserve University, Cleveland, OH) and T. E. Mitchell (Case Western Reserve University, Cleveland, OH). J. Nucl. Mater. 105, 149-158 (1982)

RADIATION-INDUCED PRECIPITATION AT THIN FOIL SURFACES IN Ni-Be ALLOYS. T. Mukai (Case Western Reserve University, Cleveland, OH) and T. E. Mitchell (Case Western Reserve University, Cleveland, OH). 40th Annual Proceedings, Electron Microscopy Society of America, ed. G. W. Bailey, Washington, DC, 1982, pp. 598-599

THE TOP SILICON LAYER OF SOI FORMED BY OXYGEN ION IMPLANTATION. R. F. Pinizzotto (Texas Instruments, Inc., Dallas, TX), B. L. Vaandrager (Texas Instruments, Inc., Dallas, TX), S. Matteson (Texas Instruments, Inc., Dallas, TX), H. W. Lam (Texas Instruments, Inc., Dallas, TX), S. D. S. Malhi (Texas Instruments, Inc., Dallas, TX), A. H. Hamdi (North Texas State University, Denton, TX), and F. D. McDaniel (North Texas State University, Denton, TX). 1982 IEEE Conf. on the Application of Accelerators in Research and Industry, ed. J. L. Duggan and I. L. Morgan (Proc. Conf., North Texas State University, Denton, TX, November 8-10, 1982), IEEE Trans. Nucl. Sci. NS-30(2), April 1983, pp. 1718-1721

Submitted Papers

ULTRASTRUCTURAL AND MICROANALYTICAL RESULTS FROM ECHINODERM CALCITE: IMPLICATIONS FOR BIOMINERALIZATION. David F. Blake (University of Michigan, Ann Arbor, MI), Lawrence F. Allard (University of Michigan, Ann Arbor, MI), and Donald R. Peacor (University of Michigan, Ann Arbor, MI). Submitted to Nature

STUDIES OF GRAIN BOUNDARY CAVITATION BY SMALL ANGLE NEUTRON SCATTERING. J. G. Cabanas-Moreno (Northwestern University, Evanston, IL), M. S. Yang (Northwestern University, Evanston, IL), J. R. Weertman (Northwestern University, Evanston, IL), M. Roth (Institut Laue-Langevin, Grenoble, France), Z. Y. Zhang (Institut Laue-Langevin, Grenoble, France), G. D. Wignall (Oak Ridge National Laboratory, Oak Ridge, TN), and W. C. Koehler (Oak Ridge National Laboratory, Oak Ridge, TN). To be published in Fatigue Mechanisms: Advances in Quantitative Measurement of Physical Damage, ed. J. Lankford, D. L. Davidson, W. L. Morris, and R. P. Wei, ASTM STP 811, American Society for Testing and Materials, Philadelphia, PA, 1983

MICROSTRUCTURAL CHARACTERIZATION OF DOPED DICALCIUM SILICATE POLYMORPHS. A. Ghose (University of Illinois, Urbana), S. Chopra (University of Illinois, Urbana, IL), and J. F. Young (University of Illinois, Urbana, IL). Submitted to J. Nucl. Mater.

MICROSTRUCTURAL DEFECTS IN LASER RECRYSTALLIZED, GRAPHITE STRIP HEATER RECRYSTALLIZED, AND BURIED OXIDE SILICON-ON-INSULATOR SYSTEMS: A STATUS REPORT. Russel F. Pinizzotto (Texas Instruments, Inc., Dallas, TX). Submitted to J. Cryst. Growth

DIRECT OBSERVATIONS OF THE EFFECT OF HYDROGEN ON THE BEHAVIOR OF DISLOCATIONS IN IRON. T. Tabata (University of Illinois, Urbana, IL) and H. K. Birnbaum (University of Illinois, Urbana, IL). Submitted To Scr. Metall.

Topical Bulletin/Announcement

HIGH VOLTAGE ELECTRON MICROSCOPY

Division of Material Sciences, Office of Energy Research, DOE, Information Exchange, Limited Distribution

ANL/HVEM-84-1 January 1984

Seventh International Conference on High Voltage Electron Microscopy

K. L. Merkle and K. Westmacott

The 7th International Conference on High Voltage Electron Microscopy which was held at the Lawrence Berkeley Lab., Berkeley, CA, August 16-19, 1983, brought attention to several major advances in the field of High Voltage Electron Microscopy. Particularly noteworthy are the advances in instrumentation that have been made since the previous HVEM conference. The higher resolution that is theoretically possible due to the shorter wavelength of high energy electrons has now been realized in several HVEM's. This promises to be a major impetus to the field since the point to point resolution is pushed towards and below the shortest interatomic distances that typically occur in solids. In addition, the advantages of HVEM's are being increasingly exploited not only for the structural, but also for the chemical microcharacterization of solids. Many of the scientific papers presented at the Conference focussed on High Resolution and In-Situ Experimentation. Important results, only obtainable thorugh in-situ HVEM experimentation, were presented from several fields such as radiation effects, phase transformation, and mechanical deformation in metals and ceramics. It became apparent that the HVEM also has become an important research tool for a number of industrial applications. At the conclusion of the Conference participants had an opportunity to visit the newly installed Atomic Resolution Microscope at the Lawrence Berkeley Lab. This is a state of the art installation that has already exceeded technical expectations in several respects and promises to be a very exciting research tool for High Resolution HVEM studies. The proceedings of the conference are published as LBL-16031, UC25, Conf-830819 which is available from the National Technical Information Service, U. S. Department of Commerce, 5285 Port Royal Road, Springfield, VA 22161.

During the Conference, several U.S. users of AEI/KRATOS HVEM's had an informal discussion regarding the exchange of technical information on their instrumentation and instrumental improvements. The establishment of a users group was discussed and it was felt that a regular exchange of information among U.S. users, similar to the practice in the U.K. and Europe, would be of considerable benefit to the U.S. installations. A summary report follows.

Summary of U.S. AEI/KRATOS HVEM Users Group Meeting

William F. Tivol

Problems: Berkeley has had many problems due to flaws at installation: accelerator sections were not all functional, anode would not lower as it should, SF_6 leaked, the beam occasionally moves off-screen, and difficulties sustaining maximum voltage. This last problem is also present at other installations; the conditioning voltage is only 40 or 50 kV higher than maximum voltage. Ni-Cd batteries give everyone some problems with shelf life and/or bad batteries shipped. Wisconsin uses a DC-DC converter and has had excellent results for over 2½ years. Filament lifetime discussions reached the consensus that good accelerator vacuum, no over-saturation, and proper positioning in the Wehnelt are critical to long life; AGAR and EBTEC filaments have been found to be good and AEI filaments are not. Berkeley had an intermittent problem with P1 which turned out to be a contact problem. Wisconsin has modified objective lens astigmatism and focus controls. They are a great improvement. Berkeley has improved the heating stage. Phosphor screens, image intensifiers and the viewing window were discussed as was the desire for more information (magnification, camera length, etc.) on negatives. The Martinaire valves give problems at all installations. Wisconsin has used DC coils and DC fans which give longer life and lower stray fields.

Spare parts inventories: Albany has computerized their spare parts list and will send copies to the other installations. Berkeley has many spares, but there may be compatability problems with the older installations.

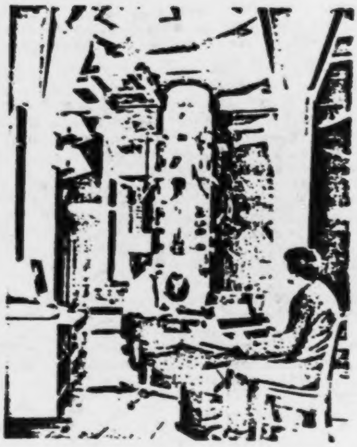
Future: Transcripts of notes of meeting will be sent to all installations. The next meeting will be by conference call about March, 1984. Six-month reports will be prepared by all facilities and sent to other facilities prior to the meeting.

BERKELEY NCEM PROGRAM

In spite of adverse winter rains, development of the NCEM has progressed with minimal delay. The ARM Support Laboratory is scheduled for acceptance in August to complete the construction phase of the project. By this time the ARM will have completed its acceptance tests and both high voltage microscopes will be in full operation.

Atomic Resolution Microscope (R. Gronsky)

The acceptance tests for the ARM are now in progress. They consist of a battery of simple calibrations (camera lengths, magnifications, etc.), a number of more tedious measurements (electronic stabilities, computer controls) and an exhaustive evaluation of resolution performance over all voltages and specimen positions (height) within the objective. These should be completed shortly, with fine tuning of specific controls (e.g. stigmator zoom, specimen stage-handling software) to follow. Attention is also being given to the final finishing of the microscope room (Fig. 1) for convenience of operation.



Measurements of the vibration isolation system for the ARM indicate that it has a natural frequency of 1.2Hz and its damping capabilities are excellent. In addition, an elaborate water-chiller recirculation system is currently being designed to provide cooling for the microscope.

By all indications, the Atomic Resolution Microscope should be ready for user operation when the support laboratory is available.

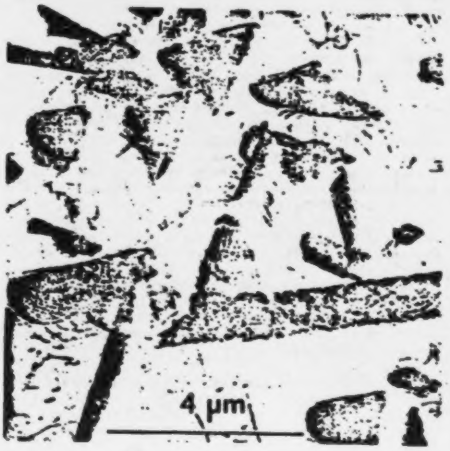
1.5 MeV High Voltage Electron Microscope (K. H. Westmacott)

A steady deterioration in the high voltage stability in the months after acceptance of the HVEM led Haefely to the decision to rebuild the bleeder resistor chain assembly. The present streamlined unit did not have the hoped-for long term stability forcing a return to the well-tested earlier design. Installation of the new parts, now in progress, should be completed within 2 weeks and is expected to return the microscope to its original performance.

Since the New Year, operation has been limited to voltages no greater than 1200kV but this has not adversely affected many of the research programs.

A new Gatan liquid nitrogen double-tilt cooling stage is now available and its performance in terms of specimen drift and temperature stability is most impressive. Many users have taken advantage of the capabilities for in-situ dynamic studies, and following some initial teething troubles, the stages are now working extremely well. The video system, donated by Bob Glaeser, is also working well and providing excellent quality recordings of dynamic events.

An example of the microstructural detail observed during in-situ heating experiments is shown in Fig. 2. In the thick foils observable in the HVEM, the formation of ' plates in nitrogen-ferrite occurs concurrently with the dissolution of α'' precipitates. Detailed observation of the development of precipitate interfacial and matrix dislocation structures is elucidating the transformation mechanisms in this and other alloy systems (work with P. Ferguson and U. Dahmen).



The excellent penetration at voltages in the range 1-1.5MeV is being exploited by users studying defect structures in electronic materials. Fig. 3 is an example of a cross-section of an MOS device taken by Tom Cass (H.-P.) and illustrates defect structures observable at the interfaces in thick sections.

ANALYTICAL MICROSCOPY WITH THE HVEM

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Analytical microscopes operating in the 100-200 keV region are fundamentally limited mainly because of multiple scattering for both x-ray and electron energy loss spectroscopies. The major drawback when considering the application of our high voltage microscope to analytical problems is the relatively large probe diameter (~100 nm) available in this instrument. Nevertheles, sufficient applications do exist at high voltages to consider in detail the advantages of this regime. In order to use x-ray spectroscopy at these high voltages, one needs to consider the use of conventional lithium-drifted silicon, intrinsic germanium or combinations of both detectors to yield a wide range of x-ray analysis capabilities; one must also consider the relativistic expression for the total ionization cross-section and the x-ray production as a function of microscope voltage. Figure 1 shows the total cross-section as a function of accelerating voltage as calculated and experimentally determined. The dashed line is calculated using an incorrect relativistic model to the cross-section expression, while the solid line was obtained using a more recent formulation. It is important to note that the total cross-section levels out at high voltages.

The situation is similar for electron energy loss spectroscopy (EELS). The intensity of the selected species is dependent upon the ratio of the sample thickness to the accelerating voltage through the mean-free path for inelastic scattering. The two methods are somewhat comlimentary in the low Z region; X-ray analysis is sample thickness limited, due to adsorption, while EELS can accommodate larger thickness with increased accelerating voltage.

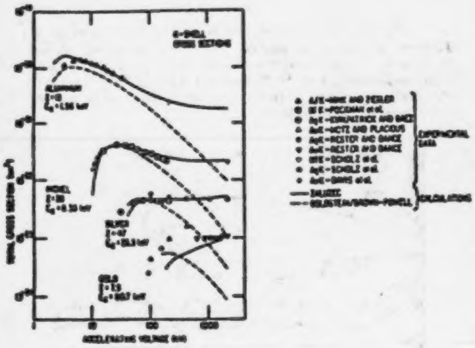

Fig. 1. Comparison of experimental and calculated x-ray cross-sections for Al, Ni, Ag and Au versus accelerating voltage.

Currently, we are in the process of designing an appropriate x-ray detector and shielding, and fitting a $\pi/2$ magnetic-sector energy analyser to the ANL HVEM.

Publications

IN-SITU STUDIES OF CASCADE DEFECT FORMATION AT T < 10 K. K. Haga (Northwestern University, Evanston, IL), A. C. Baily (Northwestern University, Evanston, IL), Wayne E. King, K. L. Merkle, and M. Meshii (Northwestern University, Evanston, IL). Proc. Seventh International Conference on High Voltage Electron Microscopy, Lawrence Berkeley Laboratory, University of California, Berkeley, CA, August 16-19, 1983, ed. R. M. Fisher, R. Gronsky, and K. H. Westmacott, LBL-16031 (June 1983), CONF-830819, pp. 139-144

IN-SITU OBSERVATION OF THE ENERGY DEPENDENCE OF DEFECT PRODUCTION IN Cu AND Ni. Wayne E. King, K. L. Merkle, A. C. Baily (Northwestern University, Evanston, IL), K. Haga(Northwestern University, Evanston, IL), and M. Meshii (Northwestern University, Evanston, IL). Proc. Seventh International Conference on High Voltage Electron Microscopy, Lawrence Berkeley Laboratory, University of California, Berkeley, CA, August 16-19, 1983, ed. R. M. Fisher, R. Gronsky, and K. H. Westmacott, LBL-16031 (June 1983), CONF-830819, pp. 133-138

THRESHOLD ENERGY SURFACE AND FRENKEL PAIR RESISTIVITY FOR Cu. Wayne E. King, K. L. Merkle, and M. Meshii (Northwestern University, Evanston, IL). J. Nucl. Mater. 117, 12-25 (July 1983) (Proc. TMS-AIME Fall Mtg., St. Louis, MO, October 24-28, 1982)

EXPERIMENTAL DETERMINATION OF THE ENERGY DEPENDENCE OF DEFECT PRODUCTION. K. L. Merkle, W. E. King, A. C. Baily (Northwestern University, Evanston, IL), K. Haga (Northwestern University, Evanston, IL), and M. Meshii (Northwestern University, Evanston, IL). J. Nucl. Mater. 117, 4-11 (July 1983) (Proc. TMS-AIME Fall Mtg., St. Louis, MO, October 24-28, 1982)

SURFACE SEGREGATION MEASUREMENTS DURING ELECTRON IRRADIATION. T. Muroga, P. R. Okamoto, and H. Wiedersich. Radiat. Eff. Lett. 68(6), 163-167 (February 1983)

RADIATION-INDUCED MICROSTRUCTURAL CHANGES IN Ni-C AND Pt-C ALLOYS. P. G. Régnier (CEN, Saclay, France) and N. Q. Lam. Dimensional Stability and Mechanical Behaviour of Irradiated Metals and Alloys (Proc. Intl. Conf., Brighton, England, April 11-14, 1983), British Nuclear Energy Society, London, 1983, pp. 51-54

MICROSTRUCTURAL TRANSITIONS IN Pt-C ALLOYS DURING HIGH-VOLTAGE-ELECTRON-MICROSCOPE IRRADIATION. P. G. Régnier, N. Q. Lam, and K. H. Westmacott (Lawrence Berkeley Laboratory, Berkeley, CA). J. Nucl. Mater. 115(2&3), 286-296 (April 1983)

RECENT WORK USING THE ANL HVEM-ION BEAM INTERFACE. A. Taylor and E. A. Ryan. 1982 IEEE Conf. on the Application of Accelerators in Research and Industry, ed. J. L. Duggan and I. L. Morgan (Proc. Conf., North Texas State University, Denton, TX, November 8-10, 1982), IEEE Trans. Nucl. Sci. NS-30(2), April 1983, pp. 1263-1265

An increasing fraction of the facility use is by biologists (~15%). The ability to obtain stereographic pairs from thick sections is particularly useful in helping to interpret large complex biological structures.

Publications and Presentations

"Periodic Extension in Optical Diffraction Analysis", R. Gronsky and C. S. Murty in Proc. 40th Ann. Meeting Elec. Micros. Soc. Amer. Washington, D. C., G. W. Bailey (ed.), Claitors, 1982, p. 428.

"High Resolution TEM of Sintered AlN", G. Van Tendeloo and G. Thomas, ibid., p. 546.

"Real Space Image Simulation in High Resolution", R. Kilaas and R. Gronsky, Ultramicroscopy (in press).

"National Center for Electron Microscopy", K. H. Westmacott, R. Gronsky and G. Thomas, AIME Fall Meeting, St. Louis, Mo., October 26, 1982.

"Defect Clustering Induced by Secondary Collisions in Pt(C) Alloys during HVEM Irradiation", by P. Regnier, N. Q. Lam and K. H. Westmacott, Scripta Met. 16, 643 (1982).

"Loss of Coherency of Precipitates in Al-Si: An HVEM Study", by K. H. Westmacott and U. Dahmen, Proc. 40th Ann. Meeting Elec. Micros. Soc. Amer. Washington, D. C. 1982. G. W. Bailey (ed.) p. 620.

"Invariant Line and Loss of Coherency in Mo(C) Systems", J. M. Lang, ibid., p. 622.

"A Novel Method for Analyzing Phase Transformations from Diffraction Patterns", U. Dahmen and K. H. Westmacott, 10th Int. Congress on Electron Microscopy, Hamburg, August 1982.

"A Study of Precipitation in Interstitial Alloys: IV. The Precipitation Sequence in Pt-C", K. H. Westmacott, M. J. Witcomb and U. Dahmen, Acta Met. 31, 755 (1983).

"The Origin of Mo_2C Precipitate Morphology in Molybdenum", J. M. Lang, U. Dahmen and K. H. Westmacott, phys. stat. sol. (a) 75, 409 (1983).

"Characterization and Structure of Intergranular Glassy Phases in Ceramics", J. Y. Laval, K. H. Westmacott and M. C. Amamura, 5th Int. Cong. on Physics of Non-Crystalline Solids, Montpellier, France (1982).

"Life Beyond 1 MeV", K. H. Westmacott, Prakt. Met. 19, 474 (1982).

ARGONNE NATIONAL LABORATORY PROGRAM

DISPLACEMENT CASCADE COLLAPSE IN Cu_3Au AT LOW TEMPERATURES

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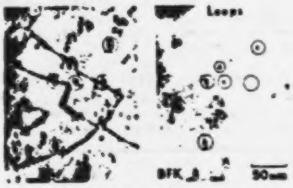
This experiment was designed to gain information on the important but poorly-understood mechanism by which the vacancy-rich cores of displacement cascades collapse to dislocation loops. The aim was to make direct measurements of defect yield (defined as the proportion of cascades which collapse to loops visible in the electron microscope) at low irradiation temperatures.

Thin-foil specimens (thickness t < 30nm) of well-ordered Cu_3Au were prepared by vacuum evaporation at the University of Oxford. These were irradiated *in situ* at controlled temperatures T < 30K in the liquid helium stage of the unique HVEM-Tandem Facility at Argonne National Laboratory, comprising an AEI EM7 microscope interfaced to a heavy-ion accelerator. The ions included Ar^+, Cu^+ and Kr^+, ranging in energy from 50 to 100keV, and the dose was typically ~ 2.10^{15} ions m^{-2}. The microscope was operated at 300 keV, below the threshold for electron irradiation damage in Cu_3Au. Experiments to allow direct determinations of defect yield, independent of the accuracy of the dose measurement, were carried out as follows. The same area of the specimen was imaged at T ≅ 10K and after warm-up to room temperature under each of the following conditions:

(i) Dark-field using a strongly excited superlattice reflection $g = \{110\}$. In this imaging condition disordered zones, which are formed at *all* displacement cascade sites are rendered visible.

(ii) Dark-field using a strongly excited fundamental reflection $g = \{220\}$ and bright-field kinematical with $\{220\}$ reflections contributing to the image. Under these imaging conditions dislocation loops, which are present at *some* cascade sites, are revealed.

Figure 1 displays an example of this defect yield at T ≅ 10 K where the circled dislocation loops are coincident with those disordered zones that are circled. Careful comparison of images obtained under these two types of conditions allows a direct estimate of defect yield.



In-situ irradiation at low temperature
100 keV $Ar^+ \rightarrow Cu_3Au$

A preliminary qualitative analysis of our results has confirmed that under the conditions of our experiments cascade collapse *does* occur at irradiation temperatures down to T ≅ 10K. There may be a reduction in yield compared with the corresponding room temperature irradiations, but more careful quantitative analysis is required to confirm this. Such analyses, giving values of defect yields as a function of the incident ion mass and energy, are currently being carried out and some preliminary results will be reported (EMAG 83, Guildford, UK).

HIGH VOLTAGE ANALYTICAL ELECTRON MICROSCOPY. N. J. Zaluzec, A. Taylor, E. A. Ryan, and A. Philippides. Proc. Seventh International Conference on High Voltage Electron Microscopy, Lawrence Berkeley Laboratory, University of California, Berkeley, CA, August 16-19, 1983, ed. R. M. Fisher, R. Gronsky, and K. H. Westmacott, LBL-16031 (June 1983), CONF-830819, pp. 79-84

Publications by Other Users

DEFECT AGRREGATION IN IRRADIATED Ni$_3$Al AND NiAl. H. C. Liu (Case Western Reserve University, Cleveland, OH) and T. E. Mitchell (Case Western Reserve University, Cleveland, OH). J. Nucl. Mater. 107, 318-326 (1982)

DEFECT STRUCTURES IN β-NiAl AND THEIR RESPONSE TO ELECTRON IRRADIATION. H. C. Liu (Case Western Reserve University, Cleveland, OH) and T. E. Mitchell (Case Western Reserve University, Cleveland, OH). Point Defects and Defect Interactions in Metals, ed. Jin-ichi Takamura, Masao Doyama, and Michio Kiritani (Proc. Yamada Conf. V, Kyoto, Japan, November 16-20, 1981), Yamada Science Foundation, University of Tokyo Press, Tokyo, Japan, 1982, pp. 635-638

A HVEM STUDY OF RADIATION-INDUCED SEGREGATION IN DILUTE Ni-Be ALLOYS. T. Mukai (Case Western Reserve University, Cleveland, OH) and T. E. Mitchell (Case Western Reserve University, Cleveland, OH). Point Defects and Defect Interactions in Metals, ed. Jin-ichi Takamura, Masao Doyama, and Michio Kiritani (Proc. Yamada Conf. V, Kyoto, Japan, November 16-20, 1981), Yamada Science Foundation, University of Tokyo Press, Tokyo, Japan, 1982, pp. 950-953

NATURE OF DISLOCATION LOOPS IN ELECTRON-IRRADIATED CuAuI AND Cu$_3$Au. T. Mukai (Case Western Reserve University, Cleveland, OH) and T. E. Mitchell (Case Western Reserve University, Cleveland, OH). Phil Mag. A 45(5), 741-751 (1982)

RADIATION-INDUCED HOMOGENEOUS PRECIPITATION IN Ni-1 at% Be ALLOYS. T. Mukai (Case Western Reserve University, Cleveland, OH) and T. E. Mitchell (Case Western Reserve University, Cleveland, OH). J. Nucl. Mater. 105, 149-158

RADIATION-INDUCED PRECIPITATION AT THIN FOIL SURFACES IN Ni-Be ALLOYS. T. Mukai (Case Western Reserve University, Cleveland, OH) and T. E. Mitchell (Case Western Reserve University, Cleveland, OH). 40th Annual Proceedings, Electron Microscopy Society of America, ed. G. W. Bailey, Washington, DC, 1982, pp. 598-599

THE TOP SILICON LAYER OF SOI FORMED BY OXYGEN ION IMPLANTATION. R. F. Pinizzotto (Texas Instruments, Inc., Dallas, TX), B. L. Vaandrager (Texas Instruments, Inc., Dallas, TX), S. Matteson (Texas Instruments, Inc., Dallas, TX), H. W. Lam (Texas Instruments, Inc., Dallas, TX), S. D. S. Malhi (Texas Instruments, Inc., Dallas, TX), A. H. Hamdi (North Texas State University, Denton, TX), and F. D. McDaniel (North Texas State University, Denton, TX). 1982 IEEE Conf. on the Application of Accelerators in Research and Industry, ed. J. L. Duggan and I. L. Morgan (Proc. Conf., North Texas State University, Denton, TX, November 8-10, 1982), IEEE Trans. Nucl. Sci. NS-30(2), April 1983, pp. 1718-1721

ALBANY PROGRAM

Element Analysis on the HVEM

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A Kevex detector was specially designed for the AEI EM7 to provide variable geometry. In the extended position the detector is 16.8 mm from the specimen giving a solid angle of collection of 0.035 sr, and when fully retracted, the detector is behind the specimen ring and does not interfere with the normal operation of the microscope. A new specimen ring incorporating a removable lead shield was installed. The detector looks upward at a 15° angle to the underside of the stage, which can be tilted to optimize signal-to-noise.

A series of lead disks was installed in the upper objective pole piece. Holes in the centers of the disks are alternately equal to and slightly larger than the bore. This provides 7/8" of lead with a crenellated central hole which results in the elimination of x-ray background arising from the upper part of the column.

The other major source of background, multiple scattering within the specimen area appears to be negligible for voltages between 400 and 1200 kV in marked contrast to the situation at lower voltages. The forward peaking of the scattering and the larger bore in the lower objective pole piece apparently allows the scattered electrons and brehmsstrahlung x-rays to leave the specimen area before significant spurious characteristic x-rays are produced.

Probe-size measurements show that 75% of the beam falls in an area whose diameter is 0.42 um, and 90% of the beam in an area of diameter 0.55 um. Spectra obtained from various biological specimens demonstrate this level of spatial resolution. These measurements were obtained with the conditions routinely used for microanalysis on our instrument: a 250 um second condenser aperture, maximal excitation of the first condenser lens, an accelerating voltage of 1000 kV, and minimum gun bias voltage.

Sensitivity measurements are in progress. Theory predicts roughly an order of magnitude gain going from 100 kV to 1200 kV.

Futher information including drawings of the installation, spectra obtained from test samples, and availability of the HVEM as a regional resource are available from the authors.

This work is supported by the Department of Health and Human Services under grant number 5 R01 GM 28614-03. The New York State HVEM facility is supported as a National Biotechnology Resource under grant number RR01219.

FORMAT OF CONTRIBUTIONS TO HVEM TOPICAL BULLETIN/ANNOUNCEMENTS

Authors are requested to submit their contributions in a camera-ready format that can be reduced 30% to give a final column width of 3-1/2 in. Please conform to the following instructions: **Typeface:** IBM Prestige Elite Type or equivalent, 12 characters per in. **Column Format:** Two columns, each 4-1/2 in. wide, maximum length 12 in. (If right-sided margin justification is possible, please use it.) **Title:** Uppercase letters, singly spaced lines, keep title as brief as possible. **Authors' Names:** Double space after title, lowercase letters with first letters uppercase. **Text:** Double spaced after authors' names, singly spaced lines, double space between paragraphs, 5-space paragraph indents. **Figures:** Submit black and white prints or diagrams drawn in ink. Figures may be two columns (9 in.) wide, but single-column width (4-1/2 in.) is preferred. Figures less than 2 in. wide should be set to the left side of the column with a narrow column of text to the right. **Deadlines:** Please submit contributions at least one month prior to proposed publication months (April and November) to the editor, A. Taylor, Materials Science and Technology Division, Argonne National Laboratory, 9700 S. Cass Ave., Argonne, Illinois 60439.

The information contained herein is intended for limited distribution among HVEM users. Readers are expected to respect the rights of the authors in order to encourage early dissemination of their results. Please address all inquires regarding format of contributions

HVEM Bulletin
c/o A. Taylor, Editor
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Argonne, Illinois 60439

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2.4 Intense Pulsed Neutron Source (IPNS-I)

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

   Answer: Neutron beams can be used to obtain microscopic information on various materials, chemicals and biological samples. These materials play a vital role in our technological society, and the information obtained using neutrons can play an important role in improving the performance of materials. Neutrons have unique capabilities to give this information because of their highly penetrating nature and ability to interact with different atom species.

   The IPNS is presently the most intense and best instrumented facility in the world for exploring the scientific opportunities presented by pulsed spallation neutron sources. The immediate opportunity offered by spallation sources is the exploitation of the rich epithermal neutron spectrum. Thus experiments at IPNS designed to use short wavelength (high energy) neutrons have been of worldwide interest. The longer term aspect is whether spallation sources can in the future replace the aging research reactors in the country. To address these questions IPNS staff have designed and built new instrumentation aimed at working in the thermal and cold (low energy) end of the neutron spectrum. At this stage, after two years of operation, it is fair to say that IPNS has established itself as the leading facility in the world in both these important tasks facing spallation sources.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

   Answer: IPNS produces bursts of neutrons with a peak thermal flux of 4 x 10^{14} n/cm^{2}sec at a repetition rate of 30 Hz and is at at present the most intense pulsed source in the world. Neutrons are produced with a 500 MeV proton beam incident on a depleted uranium target at an average current of 12 microamperes. A polyethylene moderator surrounds the target to reduce the energy of the neutrons to allow neutron scattering research. Twelve horizontal and two vertical beam holes surround the moderator assembly. A cold moderator (20 K) is available for 3 of the beams. A separate uranium target is used for fast neutron irradiation and arranged so that the samples can be irradiated at liquid helium temperature. The radiation effects facility receives the beam 25% of the time, and the neutron scattering target 75% of the time.

   Accelerator modifications and installation of an enriched uranium target are planned over the next two years to significantly increase the intensity of IPNS.

   Almost all the instrumentation at IPNS is unique. Other smaller spallation sources that exist in the world are at Harwell (UK), at Tsukuba (Japan), and at Los Alamos. A much larger facility - the Spallation Neutron Source (SNS) - is coming on line in early 1985 at Rutherford (UK) and the Germans have proposed a very large facility (SNQ) be built at Jülich. At IPNS the chopper spectrometers and powder diffractometers exploit the unique epithermal spectrum available from a spallation source, the small-angle and single-crystal diffractometers are testing new ways of doing these measurements at pulsed sources, and both incorporate unique instrumentation; specifically, the position-sensitive scintillation detector at the single-crystal diffractometer and the use of the short wavelength neutrons on the small-angle diffractometer. The radiation effects facility is the only one of its kind at a spallation source and is performing unique research in this area, specifically exploiting the low gamma flux and the ability to control the dose rate.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

   Answer: There are seven instruments currently available in the user mode, including two high resolution powder diffractometers, a single-crystal diffractometer operating on the Laue principle with a position-sensitive detector of the scintillation type; a small-angle diffractometer, also with a position-sensitive detector; a crystal-analyzer spectrometer primarily for observing H-modes in chemical systems; and two chopper spectrometers with incident energies ranging from 50 to 1000 MeV, which allow scattering measurements over a broad range of energy and wavevector transfer. Three additional instruments are under development: a polarized neutron instrument for studying refraction from surfaces; a diffractometer built to search for ordered nuclear moment arrangements in He^3 below 1 mK; and a spectrometer using resonance absorption for spectroscopy in the eV range.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

   Answer: The research highlights have been connected with the exploitation of the available neutrons for obtaining a microscopic information on the static and dynamic properties of condensed matter. Specific areas of research include the solution of complex crystal structures, for example, zeolites, by using the high resolution of the neutron powder diffraction in FY 1981 and 1982; the examination of bulk residual stress in zircaloy bars and tungsten carbide cermets with the single-crystal diffractometer, e.g., in organic superconductors in FY 1983 and 1984. Examples of experiments in FY 1984 aimed at investigating dynamic behavior include studies of amorphous solids, e.g., SiO_2; liquids, e.g., water and molecular motions in hydrocarbons; and momentum distributions in quantum solids e.g., ^{3}He and ^{4}He. Biological experiments in FY 1984 have included the study of membranes and solution conformation scattering from rhodopsin and calmodulin. Materials science applications in FY 1984 have ranged from the study of radiation induced precipitates in alloys to the setting of concrete. Radiation damage induced by neutrons is also studied. Experiments during FY 1984 have been made in semiconductors and ordered alloys; in the latter the pulse nature of the beam has been exploited to examine dose-rate dependent effects.

   New capabilities are constantly being developed at IPNS and below are described plans for FY 1985 except for completed programs. For example, high pressure studies of interest to geophysicists will be extended to low temperature and even higher pressure. Catalytic reactions will be monitored on a real-time basis. Furnace temperatures will be extended to 1500°C to allow the study of molten salts. Polarized neutron studies of field-penetration effects in superconductors will be completed in FY 1984. Software is being developed for using the pulsed nature of the beam to study relaxation effects in metals and polymers. A unique eV spectrometer for probing the spectral region above 1 eV in metals and insulators is being developed and will be brought into operation in FY 1985.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: At startup of the IPNS (November 1981), five instruments were working. Over the last two years, six additional experimental facilities have been brought on line. The computer control has been modified and an additional VAX 11/750 will be purchased this year to supplement the already considerable capability of our VAX 11/780. At present, sixteen remote terminals are connected to the central computer. The other major initiative being pursued at this time are calculations and evaluations for the installation of an enriched (booster) ^{235}U target in IPNS. This will increase our flux by a factor of three for a cost of $500K. The studies and research connected with the initiative are being financed by laboratory discretionary funds.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer:

		(B/A in thousands)				
	Support Source	FY 1981*	FY 1982+	FY 1983	FY 1984	FY 1985
Operations	BES/MS	4929	3685	3895	4712	5066
	INDUSTRY	0	0	0	17	30
In-House research	BES/MS	1410	1690	2200	2300	2400
Out-of-house research(1)	BES/MS	0	0	400	465	540
	DOE/OTHER	N/A	350	252	895	982
	INDUSTRY	N/A	125	125	145	170
	OFA/NSF	N/A	350	400	465	540
	UNIV.	N/A	575	600	700	815
	FOREIGN	N/A	250	400	465	540
Capital Equipment	BES/MS	180	300	300	275	450
GPP		12	75	70	25	145

(1) These totals represent our estimates of the research support provided non-Argonne facility users through their home institutions for work in which the Argonne facility plays a prominent role. The conservative algorithm used here is one principal-investigator-year = $100K, one IPNS experiment = 1/4 PI year = $25K.

* The IPNS Construction Project (FY 1979 $6.4M and FY 1980 $2.4M) ended in May, 1981. Pre-operational testing continued for the remainder of FY 1981. Facility operation included instrument construction and testing, safety analyses, computer programming, etc.

+ IPNS operation began in November 1981.

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer: There has been no funding for IPNS operation by any other federal or state agency, or foreign institution. However, in two important areas of technology transfer IPNS-related activities have been funded. First, the development and successful construction of an uranium target at IPNS led the Japanese to request (in early 1982) that ANL build one for them. This contract was signed in 1983, and the target is to be delivered in late 1984 for which the Japanese are paying approximately $300,000. Second, the successful operation of the world's first neutron position sensitive scintillator detector led the Institut Laue Langevin (Grenoble, France) to contract for such a detector, which will be delivered in early 1985. The charge for this by ANL is $80,000.

8. **For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.**

Answer:

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
IPNS Staff (FTE)	49.5	48.7	48 9	50.3	50.3
Research Staff (FTE)	23.0	23.0	23.5	24.0	24.0

These IPNS figures include technical and engineering staff for facility operation, scientific staff for instrument development and program administration, and scientists within the IPNS program for user interaction. The research staff figures are scientists in the programmatic divisions (Materials Science, Chemistry and Biology) that do scientific research at IPNS and interact with IPNS users.

9. **What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?**

Answer: IPNS is restricted by its budget to run 6 months/year. ("Run" here means 24 hour/day, 7 day/week operation.) Because the system is based on an accelerator and thus requires routine maintenance, we estimate "full" utilization to be operation for 9 months/year.

Utilization factor = 6 mo./9 mo. = 67%.

10. **For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?**

Answer: In the first two years of operation (November 1981 - September 1983), about 220 experiments have been completed at IPNS. More than 50% of these have non-Argonne scientists as principal investigators. Essentially all of the earlier ones have resulted in publications. Others (~50%) are still being evaluated and written up. The users are required to file an experimental report before being granted additional beam time at the IPNS facility. A large collection of experimental reports and lists of the publications (by subject) are given in the "IPNS Progress Report 1981 - 1983," which was produced for the first User Meeting in November 1983. The larger number of user instruments should result in approximately 150 experiments being performed in each of FY 1984 and FY 1985.

11. **What is this facility's user policy?**

Answer: The user policy at IPNS is well defined and has been successfully implemented since startup in November 1981. Twenty-five percent of the beam time for each instrument is assigned to the Argonne scientist responsible for that instrument. The remaining 75% of beam time is assigned by a Program Committee (joint with WNR/PSR at Los Alamos) based on proposals submitted twice a year. The Program Committee consists of thirteen scientists, two from ANL, two from LANL and nine from outside. The chairman is also from outside the DOE laboratories. Experimenters who are allocated beam time by the Program Committee have free use of the instruments, ancillary equipment (furnaces, cryostats, high-pressure cells, etc.), data acquisition system, and technical assistance. The central computer can be accessed free from the user's home institution for data analysis and refinement. Users from North American universities can receive full travel and living support from the University of Chicago, which has also provided a car for the users. Proprietary beam time can be purchased for $2400/instrument day (24 hours). Another important factor in the IPNS user policy has been the variety of schools, workshops, and conferences that we have sponsored to inform the outside scientific community about the scientific possibilities at IPNS. No less than eleven such functions have been held since 1981. A description of them is in the IPNS Progress Report. A total of 825 scientists have attended these functions.

12. **For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?**

Answer:

	(B/A in Thousands of $)				
	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Reimbursable Work	0	0	0	17*	30**

* Schlumberger-Doll Research

** Schlumberger-Doll work will continue. Also, contract negotiations are in procress with three other industrial laboratories. This number is a lower limit.

13. **What is the mechanism by which specific research proposals for experiments at the facility are considered?**

Answer: Scientists submit proposals (a short two page document) describing the work they wish to perform The scientific case is then judged by the Program Committee. The Program Committee consists of thirteen scientists, two from ANL, two from LANL, and nine from outside. The chairman is also from outside the DOE laboratories. This committee meets every six months; a proposal deadline is announced in advance. The program committee meets one month after the proposal deadline and experimenters are notified of the committee's decision within two weeks.

14. **How many research proposals have been submitted over the past five years, and how many of these have been approved?**

Answer: The number of proposals submitted over the last two years (since IPNS started operation) has been 425. Of these, 270 have been approved.

Since we are a new operation, it is also of interest to examine the growth of proposals over the last two years. In the last round of proposals, 101 were submitted requesting 760 "instrument days" of neutron beam time. The Program Committee was able to allocate 300 "instrument days" representing a rejection rate of 60%. In the latest round, 185 different scientists from 70 different institutions were involved in the proposal process.

15. How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?

Answer:

Actual university-based users for FY 1982 and FY 1983	=	88
Estimated university-based users for FY 1984 and FY 1985	=	106
Total		194

These numbers represent people who physically came to the facility and performed an experiment. A much larger number is attained by counting all collaborators. This remark applies to questions 16 and 17 as well. Once again the university participation has been increasing strongly. In the last round, 300 instrument days were requested by university investigators alone, and many more were involved in collaborative investigations with ANL personnel. The university participation, especially of graduate students, has been considerable in our variety of workshops and schools. Over 450 university scientists have attended.

16. How many industrial researchers have utilized the facility over the past five years?

Answer:

Actual industrial users for FY 1982 and FY 1983	=	10
Estimated industrial users for FY 1984 and FY 1985	=	11
Total		21

We have a collaboration (participating research team) with Schlumberger-Doll, and expect to sell proprietary beam time to Exxon, Sohio, and possibly Amoco and IBM.

17. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer:

Actual foreign users in FY 1982 and FY 1983	=	26
Estimated foreign users in FY 1984 and FY 1985	=	37
Total		63

Since IPNS is the world's most intense spallation source, there has been much interest from the international community.

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: None. ("Researchers from other agencies" are defined as regular employees of agencies, federal or state, other than DOE or GOCO contractors.) It should be noted that IPNS accommodates about 10 users per year from other DOE laboratories.

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

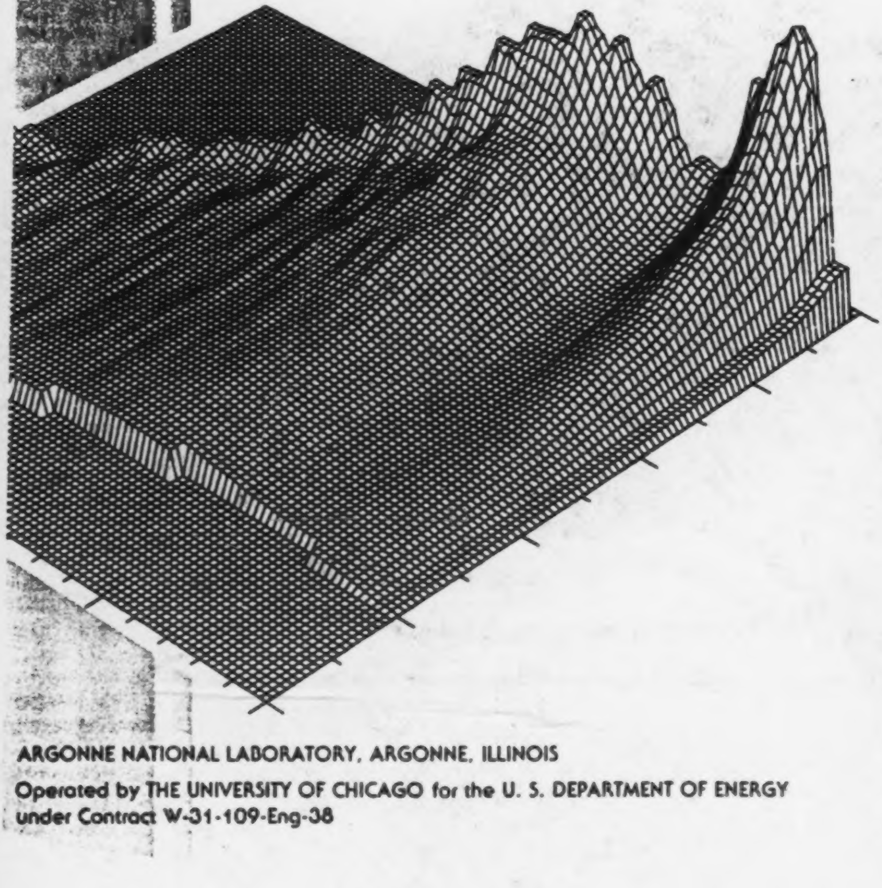
Answer: IPNS is a prototype facility with peak thermal neutron flux of 4×10^{14} n $cm^{-2}s^{-1}$. There are many potential future development possibilities for the existing IPNS facility, but there are currently no specific plans to undertake any of them beyond the activities identified in the FY 1985 budget request.

20. Please provide a copy of the facility's latest annual report.

Answer: Enclosed is a copy of the "IPNS Progress Report 1981 - 1983." More are available from the IPNS Program Office. [Note: Excerpts from this report are attached.]

IPNS

PROGRESS REPORT 1981-1983



ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS
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under Contract W-31-109-Eng-38

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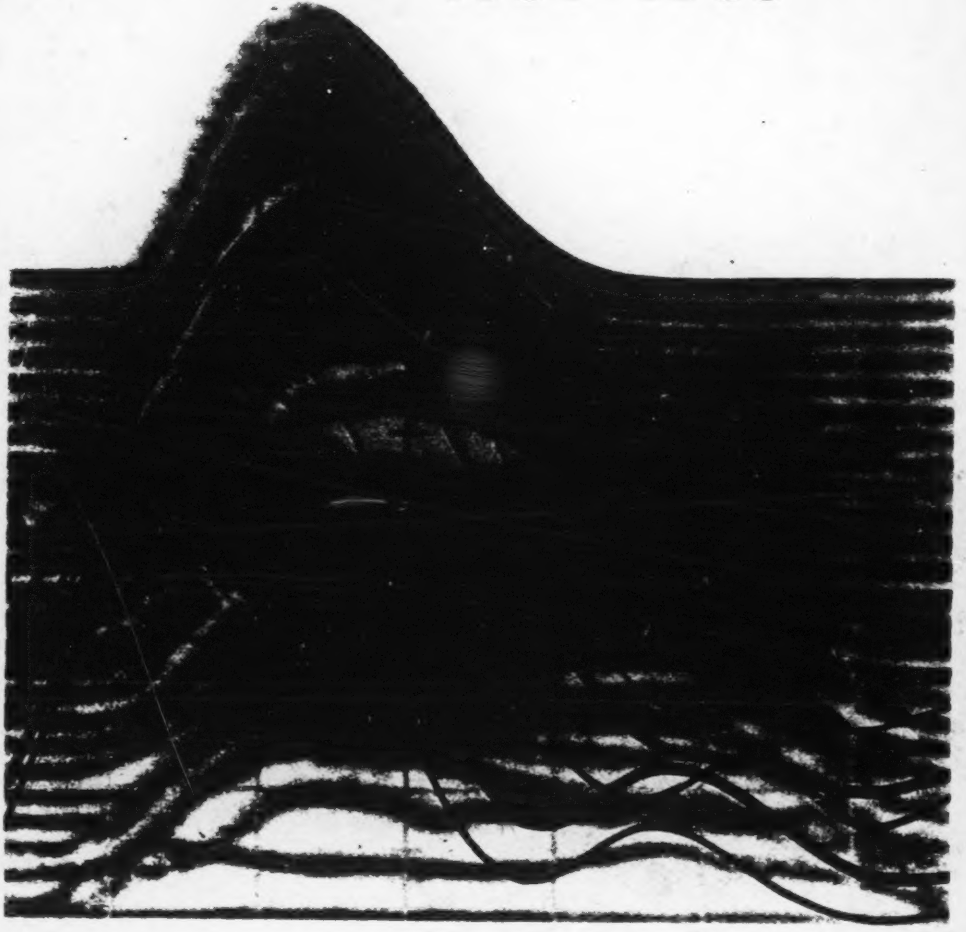
IPNS

PROGRESS REPORT

1981 - 1983



FRONT COVER PICTURE

Superposition of (i) photograph of color TV monitor showing a portion of the TOF Laue pattern for a single crystal of $K_{0.26}WO_3$, and (ii) the neutron weighted G(Q,E) from supercooled water (−20°C).

DESIGNS USED ON PRECEDING PAGE

Proton bunch lengthening by using a harmonic cavity during acceleration. Radial distribution functions for the rhodopsin-detergent complex with varying sucrose concentration in 100% D_2O.

The design at the end of Section 1 is due to D. Hulet of the Energy and Environmental Systems Division, ANL.

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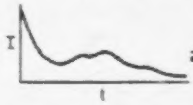

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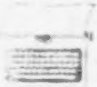

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Foreword

In the large hall that houses the research instruments at IPNS stands a small neutron chopper that turns now only for visitors. Designed over forty years ago by the great Enrico Fermi, this first chopper was used at the CP-2 reactor and opened up new opportunities in neutron spectroscopy. The presence of this famous exhibit at IPNS reminds us of the long association and leadership of The University of Chicago and Argonne National Laboratory in neutron research. IPNS is today the world's most intense pulsed neutron source, and the results obtained there are of worldwide interest, for their scientific implications as well as for the development and exploitation of such sources. Much of that research and the innovative ways to use pulsed neutrons are highlighted in this Progress Report.

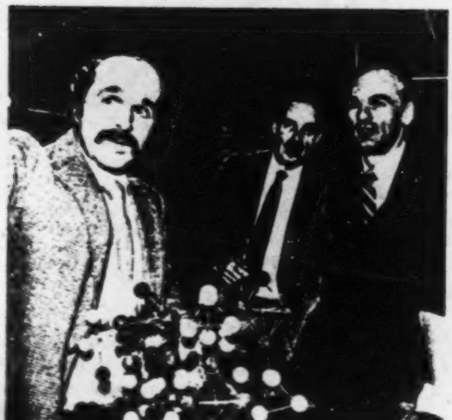
IPNS has done more than just new research. From its inception it has been operated as a National User Facility, and the large number of university, industrial, national laboratory, and also foreign scientists who are applying for time attests to the success of this policy. Such an open policy is of particular importance to the United States to enable full and imaginative use of neutron capabilities, and we are delighted to have had a central role in fostering these new attitudes. The fact that there are sufficient users to have a users meeting (the first of which is scheduled for November) points up the success of this venture!

Not content with the past and present, we at Argonne are planning for the future. Just as IPNS was envisioned after the world's first proton spallation source, ZING-P constructed at Argonne in 1974, we are now planning for a much more intense source employing imaginative accelerator technology. New instruments are also planned, to further diversify the neutron research.

Perhaps we cannot achieve the creativity of Fermi, but we can aspire to his vision!

Walter E Massey
Director
Argonne National Laboratory
October 1983

Energy Secretary D. P. Hodel visited Argonne on February 16, 1983. He is pictured here on the right, talking with IPNS Operations Manager B. S. Brown (left), and is accompanied by R. H. Bauer, Manager of the Department of Energy Chicago Operations Office.



Presidential Science Advisor G. A. Keyworth visited IPNS on April 17, 1982. Shown here (left to right) are G. Lander, G. Keyworth, D. Pewitt (assistant to Keyworth), Deputy Laboratory Director E. Beckjord, Laboratory Director W. Massey and J. Carpenter.

Introduction

The first neutrons were generated in the IPNS target in May 1981, the first neutron scattering experiments in August 1981, and the start of the formal user program in November 1981. In the two years since that time we have provided approximately 6500 hours for neutron research and the number of experiments conducted exceeds 250. This report reviews the IPNS facility over the past two years and discusses many of the important experiments that have taken place. Experimental reports, submitted after an experiment has been completed, but often before a complete analysis of the results is available, are included as an Appendix to this report. They should not be quoted without permission of the authors.

On November 15-16, 1983 we will be hosting the first IPNS — User Meeting at Argonne. Perhaps this is an appropriate point to briefly review the progress of neutrons and the user concept at Argonne over the last decade.

It is in fact just that long since pulsed neutrons were first proposed at Argonne, by Jack Carpenter, now IPNS Technical Director, and at that time on sabbatical at ANL from the University of Michigan. In 1974 the test facility named ZING-P was operated successfully and this was also the first production of neutrons for scattering experiments with a proton accelerator. More tests on a better instrumented source ZING-P' also proved successful and the idea was born to construct a major source using parts of the high-energy physics (ZGS) facility. The latter closed down in 1979, the same year the Argonne research reactor CP-5, which had operated since 1954, ceased operation, and the construction of proton transport line, target and shielding systems, and instruments for IPNS were authorized. Plans were also laid for a much more ambitious project IPNS-II, that would again use the high-energy facilities and accelerator expertise at Argonne.

In 1980 IPNS and Argonne received news that a panel (The Brinkman Panel) had been summoned by DOE to review the neutron scattering effort at the National Laboratories and recommend what to do "constrained by the likelihood that total DOE funds for neutron scattering research will not increase in terms of constant dollars." The Brinkman Panel argued strongly for an increase in total support for neutron scattering, but, if this was not possible, recommended terminating IPNS in 1983. The latter decision was affirmed in a letter to the Argonne Director of March 1981. The start up of IPNS was therefore clouded by considerable uncertainty. After seven months operation a new panel (again with W. F. Brinkman as Chairman) visited ANL and praised the science emerging from and planned at IPNS, and the beginnings of a vigorous user program. They recommended an extension of our operation, a recommendation that was followed by the funding agency.

The shadow of these decisions has to a great extent passed on by. The interested historian will find a fuller description in Science Magazine 211 (1981), p. 259; 217 (1982), p. 922 but our attention has now firmly returned to developing the best neutron research we can with pulsed neutrons, and building a user community with interest in, and access to, pulsed neutrons. Readers can be their own judges of how well we have done in these two areas from this Report.

After two years of operation and experience with pulsed neutrons it is not surprising that a number of improvements in the present instruments can be identified. Some of these improvements are discussed briefly. Accelerator improvements continue to occur at IPNS and in the longer term we have proposed building at Argonne an accelerator of a radically new design that will hopefully lay the groundwork for a dedicated $>10^{17}$ n cm^{-2} s^{-1} facility in the next decade.

Let me add a word on the organization of IPNS within Argonne National Laboratory, since this is a point that often confuses outsiders. IPNS is a facility and almost all the ~50 personnel in the program are concerned with producing first protons, then neutrons, and then assisting in all facets of data acquisition and analysis. The majority of neutron scientists at Argonne are not in the IPNS organization but belong to one of a number of scientific divisions. Of course, there is a continuous dialogue across these "virtual" boundaries, and it means that ANL scientists interact both with the neutron facility and with the many and diverse research activities on condensed matter at ANL.

In closing I should like to acknowledge the many people at IPNS who have contributed to its success, in particular David Price, my predecessor, who led the IPNS project for many years, the Accelerator and Operations groups who have had to tackle many new problems, including sociological ones associated with running the first pulsed source with a substantial outside user involvement! It is a pleasure also to thank Ken Kliewer and Walter Massey of the Argonne administration for their strong support and encouragement.

G. H. Lander
Program Director
October 1983

Pictured informally at the ICANS-VII reception are J. Carpenter, D. Price, R. Fluharty (Universal Radiations) and Associate Laboratory Director for Physical Research K. Kliewer.

Accelerator Staff, from left to right, are A. V. Rauchas, F. R. Brumwell, J. H. Norem, and C. W. Potts (1981).

Awards

In 1982, Jack Carpenter, the IPNS Technical Director, received a University of Chicago Distinguished Performance Award for his outstanding contributions towards the development and use of pulsed neutron sources in condensed matter science.

Jim Jorgensen of the Materials Science and Technology Division, and Mike Strauss and Raul Brenner, both of the Electronics Division, also received Distinguished Performance Awards in 1983.

Jorgensen was recognized for his work in determining the crystal structures of a variety of substances using the Time-of-Flight neutron diffraction method.

Brenner and Strauss were jointly honored for their invention of a neutron scintillation detector which senses where on the face of the detector the neutron was absorbed. It was the first basic innovation in neutron position detectors in over a decade (see Section 4).

This device also gained Argonne its twenty-seventh IR-100 Award in September 1983 — this award is presented annually by Industrial Research and Development magazine for the top 100 new technical products of the year.

1. ACCELERATOR SYSTEM

2. OPERATIONS AND SAFETY

3. DATA AQUISITION

1. THE ACCELERATOR SYSTEM

INTRODUCTION

The IPNS accelerator has managed to exceed the goals set for it at the time of facility turn-on in November of 1981. The table provides some data of interest over the last two years. Proton currents have averaged 8.65 μA and beam availability has exceeded 89%. In fact, after installation of a higher current H^- ion source in February of 1983, a weekly average current of 12 μA was achieved and short-term peak currents were 13.9 μA. An accelerator magnet problem developed in the last week of May, 1983. The neutron science experiment program dictated that we wait until the scheduled August shutdown before repairs were made. This restricted beam current in the months of June and July. Despite this setback, we are confident that a 12 μA average current will be routine in 1984. We also intend to increase the proton beam energy from 450 MeV to 500 MeV. This will increase the neutron per proton yield by 18%. The accelerator gains over the last two years have been made, despite a strong and appropriate emphasis on neutron science. Only about 5% of the available accelerator operating time has been used for accelerator studies.

Accelerator Operating Summary

	Nov. 1981-July 1982	Oct. 1982-July 1983
Proton beam energy	400 MeV	450 MeV
Average beam current	8.02 μA	9.21 μA
Operating efficiency	88.9%	90.2%
Scheduled operating time	3358 h	3833 h
Available operating time	2985 h	3458 h
Total pulses on target	2.94×10^8	3.33×10^8
Total protons on target	4.44×10^{20}	6.39×10^{20}

THE ACCELERATOR SYSTEM

The basic IPNS accelerator system was designed and built by personnel associated with the Zero Gradient Synchrotron (ZGS) high energy physics accelerator. This machine produced a pulse of 12.5 GeV protons every 3.6 s. Operation of this facility for high energy physics usage ceased in late 1979 and the synchrotron portion of the facility has been dismantled. The remaining lower energy components of the ZGS system, a 750 keV Cockcroft-Walton preaccelerator, a 50 MeV Alvarez linac and a 500 MeV rapid cycling booster synchrotron (RCS) have been modified to deliver protons 30 times per second to the IPNS spallation neutron target. The layout of the accelerator system is depicted in Fig. 1.

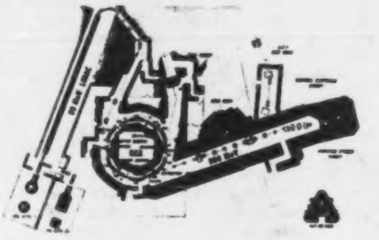


Fig. 1. IPNS Accelerator System Layout.

The proton beam originates in the preaccelerator terminal when a 40 μs burst of 1.2×10^{13} H^- ions is injected into the 750 kilovolt accelerating gap of the preaccelerator. These ions then travel through the 50-m-long linac where high frequency electric fields increase their energy. The emerging 50 MeV H^- ions are magnetically steered to the RCS synchrotron. About 25% of the ions generated in the source arrive at the synchrotron at an energy of 50 MeV.

The 40 μs burst of H^- ions passes through a 3000 Å thick plastic foil as the ions enter the synchrotron. The foil strips two electrons from each ion leaving an H^+ ion, a proton. These protons travel around the 140 ft evacuated "race track" (2 in. × 4 in. cross-section) inside the synchrotron magnets about 100,000 times in 16.7 ms. Each revolution, energy is added to this proton "cloud" by two 150 kW rf transmitters. Beam diagnostic devices automatically adjust the rate of energy addition so that despite a magnetic field increasing sinusoidally with time, the centrifugal and magnetic forces on the protons are always in dynamic balance. When it reaches full energy, the proton cloud is shaped something like a thin 56-ft-long sausage which is making a revolution around the synchrotron every 190 ns. At this point in the acceleration cycle, a very fast (90 ns) magnet is pulsed. This magnet, along with two others, steers the proton beam out of the circular synchrotron into a tangent beam transport line which, in turn, directs the proton beam toward the spallation target. The 80 ns proton burst is delivered to the target every 33.3 ms.

INITIAL OPERATION

This accelerator system ran intermittently in 1979 and early 1980 delivering protons to the ZING-P' prototype spallation target. The accelerator then produced 300 MeV proton currents averaging about 2.5 μA. The pulse rate averaged about 10 Hz. Extensive accelerator studies during this period determined the various modifications required to improve the average proton current and make a reliable 30 Hz operation possible. The accelerator was shut down for one year starting in July 1980 in preparation for beam delivery to the IPNS spallation target. During this shutdown, numerous significant accelerator hardware changes were made. Some of these are listed.

1. A new style transformer pulsed septum magnet was installed. This is a very rugged design ideally suited for 30 Hz pulsing.
2. Linac tank and transmitter cooling was increased.
3. A kicker magnet and power supply system more than twice as powerful as the old one was installed.
4. Dynamically programmable control of the lattice tune correction magnets was added.
5. The rf system was modified with additional power handling capability, improved dynamic range, and tighter control of cavity impedance.
6. Vacuum pumping was increased by 30%.
7. The computer data handling capacity was doubled.
8. The shielding over selected portions of the synchrotron tunnel was improved.
9. The beam injection and extraction apertures were enlarged.

The accelerator turned-on for neutron science on November 1, 1981. It was immediately apparent that, in the main, the equipment modifications had been beneficial; for instance, background radiation outside the synchrotron tunnel was down by a factor of 20, the beam extraction efficiency was essentially 100% and 8 μA peak currents were possible. As Fig. 2 demonstrates, within three months the goal of 8 μA average currents had been achieved. Despite a batch of faulty high voltage cables on the kicker magnet power supply, the operation was quite reliable as may be seen from Fig. 3.

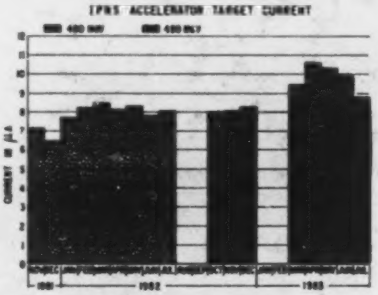


Fig. 2. IPNS Accelerator Target Current, 1981-1983.

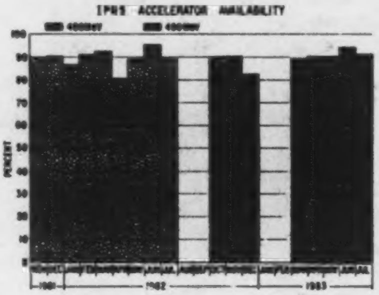


Fig. 3. IPNS Accelerator Availability, 1981-1983.

RECENT IMPROVEMENTS

The high-energy protons that strike the IPNS spallation target originate at very low energy in a device called an H$^-$ ion source located in the high voltage enclosure of the preaccelerator. As the beam handling ability of the synchrotron portion of the accelerator system was improved in 1982, it became increasingly evident that the beam current from the H$^-$ ion source was the factor limiting the number of protons striking the spallation target. Anticipating this, we had started in the fall of 1981 to adapt a 15 Hz magnetron type H$^-$ ion source to operate reliably at 30 Hz. This type of H$^-$ ion source was originally developed at Brookhaven National Laboratory and was further improved at Fermi National Accelerator Laboratory. Argonne National Laboratory's contribution was a redesign of the electrode geometry to allow lower temperature operation despite doubling the pulse rate. Installation of this new ion source was completed in February 1983 and increased current on target resulted as may be seen in Fig. 3. This ion source is capable of producing many more ions than the remainder of the accelerator system can efficiently accelerate, so it fits well with future plans to increase accelerator current. In fact, the ion source, preaccelerator and linac are capable of delivering 30 μA of 50 MeV H$^-$ ions to the RCS synchrotron.

After installation of the new H$^-$ ion source, operation resumed in March 1983. We had predicted a 25% increase in beam to 10 μA as a result of the new source. However, after only 5 weeks of operation the weekly average target current was up to 11.7 μA, an increase of 37%. Several improvements were made in the operating mode of the synchrotron to help utilize the increased 50 MeV H$^-$ ions available. The increased space charge density at injection was compensated for by shifting the "working point" with the programmable trim quadrupoles which are in the main ring lattice. A deliberate dilution of the longitudinal phase space density at mid-cycle decreased the intensity-dependent high-energy beam stability problems. Perhaps the overall key was better control of the low energy orbits. This was accomplished by improving the stability and decreasing the noise sensitivity of the high current ring magnet power supply and the high power rf transmitters.

Despite the various improvements in beam handling described above, the increased beam on target was accompanied by increased beam lost in the synchrotron. In fact, target current became limited by the amount of lost beam allowable. The synchrotron tunnel has a mean diameter of only 50 ft, a width of 7.5 ft and mean height of 8 ft. We have concluded that an average beam loss of about 5.5×10^{12} protons per pulse (2.5 μA) is the maximum loss that will still allow hands-on maintenance of accelerator equipment.

In late May, a problem occurred inside one of the synchrotron ring magnets. A necessarily hurried inspection revealed that one of the hoops of the stainless steel rf liner had been burned through and was partially obscuring the accelerating aperture in triplet magnet #6. This damage was apparently the result of protons lost. Figure 4 shows the severed piece of liner hanging down into the aperture. The mirror in this figure provides a view looking up at the melted steel and damaged epoxy.

The working area was too radioactive for complete immediate repair but a partial fix was made and the

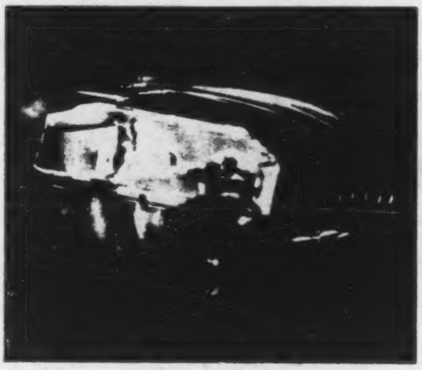


Fig. 4. Severed Piece of One of the Hoops of the Stainless Steel rf Liner, Hanging Down into the Accelerating Aperture.

scheduled science run continued. However, as Fig. 1 shows, the beam current decreased in both June and July as a result of the problem. A more detailed inspection of the inside of the synchrotron in August revealed similar damage inside another ring magnet. Both magnets will be repaired for turn-on in late September and we anticipate 12 μA capability again. Some protective adjustable carbon Faraday cups will also be installed to try to prevent a repetition of this problem.

We have, over the last two years, learned that a neutron science program has different accelerator requirements from those of a high energy physics program. In particular, synchronizing the accelerator to neutron choppers has been a challenging new requirement, which the accelerator team has worked very hard on and successfully completed. Rapid accelerator turn-on which enhances scheduling flexibility and minimizes electrical power costs has been another goal we have met. Accelerator availability, always a matter of pride on the ZGS, receives even stronger emphasis on the IPNS system. Everything considered, we feel proud of the IPNS Accelerator System Group's contribution over the last two years.

Proton Dosimetry

Cross-section measurements have been made at the Intense Pulsed Neutron Source (IPNS) at Argonne. In a somewhat unusual mode of operation for the facility, foil packages were inserted directly into the proton beam and the beam energy was lowered in steps from the normal 450 MeV down to 80 MeV. Aluminum and copper foils were then gamma counted by Ge(Li) spectroscopy to measure the yields of spallation products. Spallation is analogous to fission in that all lower mass isotopes can be produced. In the case of copper over 20 different radioactive products were identified. The goal of this research is to measure the relative yields of these products as a function of energy. With such data we expect that we can extend our neutron dosimetry to energies as high as 500 MeV. At present, such data is not known above 30 MeV. This new technique will be useful not only at spallation sources, but also will aid in the unfolding of data for Be or Li(d,n) sources, such as the FMIT under construction at HEDL, where neutron fluxes extend as high as 55 MeV.

L. Greenwood and R. Smither, Damage Analysis and Fundamental Studies Quarterly Progress Report, DOE/ER-0046/14, August 1983, pp. 19-24.

PROTON THERAPY PROGRAM

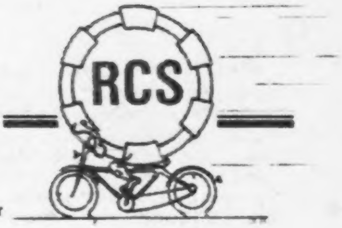
In 1946 R. R. Wilson pointed out the advantages of using the Bragg peak of the proton dose curve to enhance the tumor killing dose in radiation treatments of cancer. The medical community has been slow to respond to this technique largely because of the difficulty and cost of obtaining protons from physics accelerators, as well as the lack of experience with this radically different beam. Over the last decade significant progress toward understanding how to use protons has been taking place at Harvard University. This work has been concentrated largely on small volume tumors, where the advantages of protons are most significant. One such tumor being treated is choroidal melanomas of the eye. This relatively fast growing tumor is not successfully treated by other techniques, which usually results in a significant loss of vision or the entire eye. Treatments with proton beams have had success rates greater than 95% for tumor control with relatively good vision and low complication rates.

Ophthalmologists from the University of Illinois would like to have this treatment available in the midwest and have asked Argonne to provide the protons. Funds have been provided to make an existing 50 MeV beam available for this purpose and S. Kramer and his collaborators at Argonne are setting up the necessary equipment.

The beam to be used makes use of waste beam from the 50 MeV linear accelerator. Measurements have shown that about 1.5 nanoamperes of beam (half the intensity of the Harvard cyclotron) are available by simply opening the beam stop during routine operation of the RCS. Since the beam is not well defined, studies will be necessary to optimize the transport of this beam to the patient. During 1983 the beam was made operational; measurements and improvements will be made in 1984. These measurements will include accurate dose distribution to be made in collaboration with physicists from BIM.

Recently a team of doctors and a physicist went to Harvard to observe their treatment of these eye tumors. The goal of this trip was to gain experience and to detail the equipment necessary for treating patients. The information gathered will be used to submit a proposal in the near future to develop the necessary equipment for treating patients at Argonne. If all goes well, the first patient could be treated by the end of 1984. Although the depth of penetration of this beam is quite limited, the experience and reputation gained from treating patients with this facility will make the development of more optimized beams easier to justify.

6



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T. Worlton - Scientific Secretary/Data Acquisition Systems Manager
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T. Scott - Radiation Effects and Cryogenics
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Valuable technical help is also acknowledged from the following outside IPNS.

J. Biggs - magnet construction
G. Gunderson - computer
M. Knott - computer and control system
D. McGhee - high current power supplies
W. Praeg - power supplies and magnets

2. OPERATIONS

The IPNS Zircaloy-2 clad uranium targets have been in use in both the neutron scattering facility (NSF), see Fig. 5, and radiation effects facility (REF), see Fig. 6, since startup (1981). The depleted uranium targets consist of eight 25-mm-thick, 100-mm-diameter uranium alloy disks, clad with 0.5-mm Zircaloy-2 (1.5 mm on circumference) cooled by demineralized water flowing in 1-mm channels between the disks.

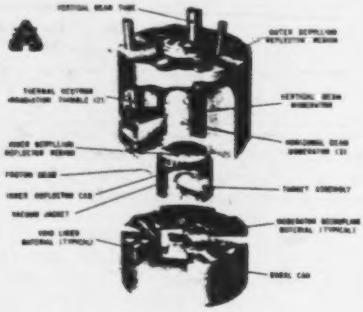


Fig. 5. Neutron Scattering Target Assembly.

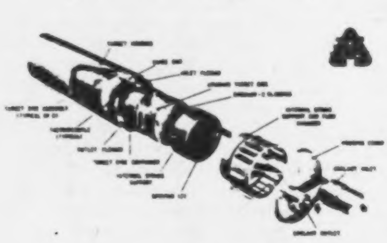


Fig. 6. Radiation Effects Target Assembly.

The neutron generating facilities and target support systems are surrounded by a biological shield which provides structural support and shielding. The biological shield consists of an inner steel shield (1100 tons) immediately surrounding the neutron generating system components and an outer concrete shield (50 tons). The steel shield is enclosed in an atmospheric control tank which functions as the boundary of the shield atmosphere control system, which is operated at slight vacuum. The shield is designed to limit radiation dose rate at any accessible location in the experimental area from all radioactive sources within the shield during normal operation to 0.5 mrem h^{-1}. The shielding also keeps the background levels at the neutron scattering instruments to a minimum.

In the neutron scattering facility, the fast neutrons produced by fission and spallation reactions in the target are thermalized by moderators (with a high hydrogen density) located above and below the target. We have used two types of moderators. One type consists of four, ambient-temperature polyethylene moderators with an inner graphite reflector. The second consists of four 100 K circulating liquid CH_4 moderators with an inner 100 K beryllium reflector. These moderators are surrounded by an outer, 300 K beryllium reflector. Twelve horizontal neutron beam tubes and one vertical neutron beam tube view selected faces of the moderators to provide neutron beams to instruments. Each horizontal beam tube contains a 36-in-thick steel beam gate. Two vertical holes (VT3 and VT4) and two horizontal holes (F-6 and H-2) may be used for sample irradiations. A polyethylene insert has been added to one of the vertical holes to enhance the neutron flux and has resulted in an increase in the thermal neutron flux by a factor of two.

In the radiation effects facility, the neutrons emitted from the target pass into high density reflector materials (lead) which maximizes the fast neutron flux within irradiation holes, two vertical (VT1 and VT2) and one horizontal. Thimbles are provided to permit samples to be inserted and removed. Two vertical tubes are equipped for irradiation of samples at controlled temperatures between 4 K and 600 K; the horizontal tube operates only at ambient temperature.

The moderator-reflector assembly used during the first year was of room temperature polyethylene with graphite reflector. This was installed to allow modification of the beryllium-reflector $L\text{-}CH_4/L\text{-}H_2$ system, which we discovered would not function as designed.

After 15 months operation, the polyethylene moderators and graphite reflector assembly was removed from the NSF during the August 1982 shutdown. The polyethylene-graphite assembly had three ambient-temperature poly moderators, with inner graphite reflector and outer beryllium reflector, and cadmium decoupling and void liners throughout. This assembly did not provide a vertical beam moderator. Upon removal of this assembly, the radioactivity levels were found to be 40 mrem h^{-1} to 120 mrem h^{-1} on the two steel shield plugs above the reflector and 200 mrem h^{-1} at 5 cm for the graphite-poly assembly.

The liquid methane moderators and inner beryllium reflector assembly was checked, tested and cycled three times using its refrigeration equipment before it was installed in the NSF. In process of testing, we found that the L-H_2 systems could not operate at 20 K while the L-CH_4 systems operated at 100 K. We decided to forgo use of 20 K L-H_2 moderators, and to operate all four moderators with 100 K L-CH_4. All tests then indicated that reliable operation could be expected. The proton beam was put on the NSF target from September 29 to October 4, 1982 (total of 2.17×10^{19} proton pulses) with a proton energy of 400 MeV. After two days of beam on target the flow to "H" moderator showed degradation, by the fourth day the flow was blocked. Various attempts to restore flow were tried including cycling the throttle valve (thought to have frozen owing to moisture), changing liquid nitrogen flow to the heat exchanger, and bypassing part of the methane flow. All attempts were to no avail. The facility was shut down and the moderator systems were warmed up. The methane gases were circulated, gas samples were taken and the methane gas was changed. The original methane charge was Grade 4.2: methane (CH_4) 99.992%, nitrogen (N_2) 20 ppm, oxygen (O_2) 4 ppm and ethane (C_2H_6) 12 ppm. The new charge was Grade 4: methane (CH_4) 99.95% and would not result in a significant change in impurity levels.

After another attempt at operating the system we decided the problem was the plugging of the 15 micron filters which were located in the weld-sealed, evacuated heat exchanger box. These filters were removed and replaced by 90 micron filters. The new filters were relocated in an accessible part of the system and fitted with easily removed slip couplings. Proton beam was again delivered to the system and flows to the 4 liquid methane moderators at 100 K were much improved. Prior to this run, we also changed the 90 micron filters to assure ourselves that we had cleaned the foreign residue from the system. Samples of the methane gas were also taken again.

From December 7 to December 21 the system ran with proton beam on target; the 4 methane moderator systems ran with no problems. A significant increase in the neutron flux was seen (factor of about 8 at 5 Å). Experiments that were run at this time indicated that the larger moderator (thicker in the direction of the neutron beam) resulted in an increase in time width of the pulse that degraded the resolution in the powder diffractometers. This led to the decision that the moderators would be reworked. During the last operating cycle on the methane system, we erected a vacuum line to test the solubility of various boron compounds in cryogenic moderator fluids to seek an easy fix to the degraded resolution problem on the powder instruments. No practical solution was found.

The room temperature polyethylene graphite beryllium moderator assembly was modified to provide a vertical moderator (LN_2-cooled polyethylene) for the ultracold neutron experiment. Also, new polyethylene moderators replaced those inserted August 1981. This system has been in operation since February 1983 till August 1983. During this summer shutdown, August-September 1983, we have built a new graphite/polyethylene reflector moderator system. The new system now has an L-N_2-cooled polyethylene moderator in the "C" position. This provides a higher intensity of long wave neutrons to the SAD, ^{3}He and polarized neutron instruments, approximately a factor of 10 at 4 Å (see Section 4).

The Neutron Generating Systems have operated without serious trouble since the start-up of IPNS. The original cold moderator system as designed would need extensive changes, especially to the liquid hydrogen moderator hardware. The available subcooling was also marginal for the liquid methane moderators. Therefore, with the prospect of an increased heating load from an enriched uranium target, a new cold moderator system will be designed and built.

SAFETY

The IPNS is considered to be a non-reactor nuclear facility by the Department of Energy (DOE), and consequently, we were required before start-up to submit a **Safety Analysis Report** (SAR), consisting of a complete analysis of the various safety systems, potential failures and their consequences, conduct of operations, user and operator qualification and interaction with Argonne safety organizations. Following approval of this document, the **Operations Safety Requirements** were generated. These consist of a series of limitations on various parameters (target temperature, coolant flow rate, etc.) which guarantee that the worst case accident analyzed in the SAR will not be exceeded. These Requirements are the limits below which IPNS must operate. Start-up approval of the DOE appraiser was given on May 4, 1981.

We continue to monitor target and cooling systems during operation, all parameters being surveyed continuously by both a hard-wired and a computer system located in the main accelerator control room.

During the entire operative period, we have not detected any significant radioactive effluents from our stack, nor any unusual radioisotopes in the cooling water. An automatic system monitors both stack emission and radioactive gaseous products in the cover gas over the cooling water. Occasional sampling of the cover gas has at no time shown any unusual build-up of hydrogen (this build-up was seen in ZING-P').

IPNS HEALTH PHYSICS

The IPNS facility provides a broad spectrum of sources of ionizing radiation, demanding comprehensive personal and environmental radiation protection. This is accomplished through a cooperative effort among IPNS Users, IPNS Operations and the Health Physics Section (HPS) of the Occupational Health and Safety Division. Specific areas of Health Physics support include area radiation monitoring and characterization, irradiated sample handling and transfer, personal dosimetry, operational testing and calibration of radiation monitoring devices, review of new projects or modifications to existing experiments, and a radiological lecture. Attendance at this orientation lecture is a prerequisite of all IPNS Users and Personnel requiring access to the Experimental Hall. Subjects covered include presentation of the facility layout and indication of locations and levels of significant sources of radiation. Procedures for handling of radioactive materials are explained and location and operation of monitoring instrumentation are discussed. All types of alarms audible from Building 375 and responses are also described. An important part of the orientation is a discussion of the interaction of Users, Operations and Health Physics both during normal working hours and during "off shift" times.

Individuals are issued with dosimetry, consisting of film badges for betas, gammas and fast (MeV) neutrons and an albedo neutron dosimeter. IPNS Users and Operations personnel together account for 150 badged individuals during a typical badge period. Except for a very few (about six) people, IPNS Users have not received any recordable exposures. The total IPNS operation represents about 10 person-rem yr^{-1}, mainly received during RCS maintenance. The highest personal exposure has not exceeded 1.5 rem yr^{-1}.

These dosage results are consistent with the exposure potential determined through area radiation monitoring and sample handling procedures. Although local spots up to 90 mrem h^{-1} (n and γ) have been measured, general radiation levels in Building 375 are less than 0.5 mrem h^{-1}. All experimental areas can therefore be accessed safely while the neutron source is up. Higher-radiation areas are posted or have barriers indicating the hazard. Hundreds of samples have been investigated at IPNS. Contact radiation measurements have indicated levels from zero to greater than 50 rad h^{-1} (β and γ). Tests for removable radioactivity from these samples have shown levels from zero to 40,000 dis min^{-1}. Sample handling operations have not resulted in any incidents of significant radioactive contamination of individuals or facilities, nor caused unreasonable external radiation exposures.

Project and operation review has played an important part in contamination containment and exposure control. These reviews range from straightforward cases of individual samples, through start-up of new

beam lines, to complex projects such as modifications to the used Neutron Scattering Facility moderator assembly. Along with HPS, the IPNS Radiation Safety Committee is an additional participant in some of these operational and modification reviews.

The various radiation monitoring devices are regularly checked by Health Physics staff who carry out any initial troubleshooting. The external radiation monitors; the cover gas activity monitor; the hand and shoe monitors; and the stack monitor have functioned well; after commissioning, these units have required little maintenance.

Neutron Activation Analysis at the IPNS

The Intense Pulsed Neutron Source (IPNS) Neutron Scattering Facility (NSF) has been investigated for its applicability to neutron activation analysis.

The challenge in using this high energy accelerator-based neutron source focuses upon knowing the neutron spectral distribution within the sample volume since neutrons of all energies are generated within the target. Thus, before meaningful activation analysis could be done, careful neutron dosimetry of the neutron spectrum had to be accomplished. The work by R. Heinrich, L. Greenwood, R. Popek, and A. Schulke indeed demonstrates that successful neutron activation analysis can be done at the IPNS facility.

A polyethylene insert has been added to the vertical hole VT3 which enhances the thermal neutron flux by a factor of two. The neutron spectral distribution at this position has been measured by the multiple-foil technique which utilized 28 activation reactions and the STAYSL computer code. The validity of this spectral measurement was tested by two irradiations of National Bureau of Standards SRM-1571 (orchard leaves), SRM-1575 (pine needles), and SRM-1645 (river sediment). The average thermal neutron flux for these irradiations normalized to a 10 μamp proton beam is 4.0×10^{11} n cm^{-2} s^{-1}. Concentrations of nine trace elements in each of these SRMs have been determined by gamma-ray spectrometry. Agreement of measured values of certified values is demonstrated to be within experiment error.

A comparison of measured SRM trace element concentrations to NBS values was made. The excellent agreement demonstrates primarily the accuracy of the neutron dosimetry and the methodology used in determining the IPNS neutron spectrum. Uncertainties on the measured values are estimated to be ±7% which includes estimated errors in the neutron cross-sections, spectrum unfolding, detector calibration, counting statistics, and neutron flux gradient corrections. Of the nine trace elements listed, only the As, Rb, and Sb appear to be biased high. This could be attributed to the reaction cross-sections used, since uncertainties for these reactions are listed at about twice as high as those for the other elements.

Conclusions are that neutron activation analysis can be successfully performed at the IPNS in the VT3 (poly) position, but this is contingent upon the fact that adequate neutron dosimetry is also provided.

3. DATA ACQUISITION

INTRODUCTION

Data collection and analysis for the nine neutron scattering instruments is accomplished using the IPNS Data Acquisition System (DAS). The IPNS DAS currently includes one VAX-11/780 computer for analysis, five PDP-11/34A computers and two PDP-11/24 computers for experiment control and histogram setup, and nine Z8001 single-board microcomputers and associated peripheral equipment. Except for a few specialized area-detector and control routines, the same software is used on all PDP-11 computers.

The IPNS DAS was designed to be reliable, flexible, and easy to use. It provides unique methods of acquiring time-of-flight neutron scattering data and allows collection, storage, display, and analysis of very large data arrays with a minimum of user input. Data can be collected from normal detectors, linear position-sensitive detectors, and/or area detectors in various combinations. The data can be corrected for time-delays and can be time-focused before being binned. Corrections to be made to the data and selection of inputs to be summed are entirely software controlled, as are the time ranges and resolutions for each detector element. Each system can be configured to collect data into millions of channels. Live displays of the data may be made as a function of time, wavevector, wavelength, lattice spacing, or energy. The complete data analysis can be done on the DAS host computer. The IPNS DAS became operational for four neutron scattering instruments in 1981 and now (1983) includes nine instruments.

SYSTEM DESCRIPTION

User Interface and Data Collection

The data collection process is controlled by DEC PDP-11 computer systems at each instrument or pair of instruments. User commands have been implemented on the PDP-11 to set up histogramming tables tailored to a specific experiment; to schedule, start, and stop data acquisition for a run or a series of runs; and to print or display data or other run information in various formats on the graphics display terminal. The PDP-11 is also used to back up the data to disk and monitor the progress of the data acquisition process and to handle various control functions.

The PDP-11 is interfaced to a MULTIBUS system containing a Z8001 single-board computer dedicated to data collection. The Z8001 microcomputer provides a system capable of addressing up to 16 Megabytes of data and executing a variety of data-histogramming algorithms while leaving the PDP-11 minicomputer free to serve as a powerful and flexible interface to the user. The data acquisition programs for the Z8001 are table-driven to allow flexibility in the formatting of the histograms. Tables are generated by routines on the PDP-11 when the user sets up the run, and are then down loaded to the Z8001 at run time.

Details about the user interface and data collection hardware, software, and overall architecture and philosophy can be found in Crawford et al. (1981), Haumann et al. (1982), Worlton et al. (1983), see Publications, Section 8, and in the IPNS DAS User Manual.

Histogramming Algorithms

The algorithm used by the Z8001 in histogramming data from standard or linear-position-sensitive detectors emphasizes flexibility, and includes the capability for on-line "time-focusing" of these detectors. This means that events from different detectors can be binned together, with events corresponding to the same d-spacing (for example) going into the same bin. Any of several variables (d-spacing, energy, wavelength) can be used as the time-focusing variable. This algorithm is table-driven, so just by changing the table, the same software can be used for all the different types of binning, channel widths, starting and stopping times, etc. used by the various instruments at IPNS.

The IPNS Data Collection software also has the unique capability of binning a given event more than once. This is equivalent to having parallel time-of-flight analyzers.

A second algorithm for area-position-sensitive detectors emphasizes histogramming speed rather than flexibility, since data rates are high and not as much flexibility is required. This algorithm is also table-driven, but the tables used in this case are much larger and provide direct mapping of the 16-bit raw-time word and the 16-bit raw-position word.

By using both algorithms and both types of parameter table, the Z8001 can handle standard beam monitor detectors concurrently with an area-position-sensitive detector.

Data Analysis

A DEC VAX-11/780 is used for data analysis and provides a variety of special software and graphics and mass-storage devices which can be shared by all instruments. Data analysis routines for all the instruments are now running on the VAX. The VAX is also linked to the central IBM computers which gives us access to additional processing power and output devices.

PERFORMANCE SUMMARY

The IPNS DAS became operational for four of the first five instruments in Summer 1981. Construction of the fifth of the proposed initial instruments was completed in 1982, and, together with four other instruments, it has been added to the DAS since it first became operational.

Data Rates

The initially established goals for instantaneous data rates have been achieved. The pulse-pair resolution for pulses in the same discriminator module is approximately 2 μs, while there is no interference whatsoever between pulses in different discriminator modules. This seems to be quite adequate for all data acquisition requirements encountered so far.

The initially established goals for time-averaged data rates have been exceeded. The DAS can handle rates in excess of 2000 events per second for non-area-detector instruments, and rates of up to 16,000 events per second for area-detector instruments. This time-averaged rate has so far proved adequate for area-detectors. However, in the case of non-area-detector instruments, some users found it desirable to make full use of the very large time-of-flight range permitted by the system. This has resulted in the data rates from these instruments (particularly powder diffractometers) being much higher than anticipated on the basis of previous experience with similar earlier instruments (which were typically restricted to fewer than 10,000 channels total for data). Data rates for these instruments are thus pressing against the limits imposed by the DAS.

Histogram Sizes

Several of the non-area-detector instruments currently have approximately 150 detectors each. In the initial calibration and testing of these instruments extensive use was made of the ability to concurrently collect and histogram data from each detector separately. The multiple-histogram option was also used extensively in this calibration/testing phase, and has been used to a lesser extent in more recent applications. Histograms (or multiple histograms) in excess of 200,000 channels have been collected on some of the non-area-detector instruments. In routine operation these instruments typically use 20,000 to 100,000 channels per run. The Single Crystal Diffractometer, which uses an area-detector, routinely collects histograms of about 800,000 channels.

Electronic Time-focusing

This concept has worked extremely well. The flexibility of the table-driven focusing algorithm was demonstrated when the chopper was removed from one of the chopper spectrometers and a time-focused powder diffraction spectrum was collected in that instrument from the same sample that was used in the inelastic scattering measurements. This required only the setup of a new run with the proper focusing parameters. In other tests on the powder diffractometers, detector banks at various angles (including angles down to about 15 degrees) have been focused with no difficulty.

Data Analysis

The presence and availability of the VAX host computer as part of the DAS have been extremely important, especially as regards experiments for outside users. Extensive data analysis software for the various instruments has been developed for the VAX by the Instrument Scientists, and this has enabled outside users to begin data analysis immediately after they have completed data acquisition, and to leave Argonne with data that have already been at least partially analyzed. This computer is quite heavily used, although the CPU is not yet saturated. It appears that our initial estimate that this computer would be nearly saturated when a full complement of approximately 12 instruments was operational at IPNS is still valid.

FUTURE PLANS

Data Collection System

We are currently working on a replacement for the single-board microcomputers which perform the actual binning of data in real-time. We plan to use the new Intel 286 microprocessor which is significantly faster than the Z8001 microprocessor now in use. The first of these new units should be available for testing in early 1984.

Another major near-term improvement to the Front End systems will be in the area of automatic data transfer to the Host Computer System through a local area network. Some features of this network are expected to be operational in early 1984.

A third area expected to be substantially upgraded in the near future is in automation of control of sample environmental parameters. Current developments are focusing on software for interfacing sample changers and temperature controllers to the PDP-11 run-control software package.

Data Analysis System

All IPNS Users are now doing data analysis on the VAX-11/780 Host Computer and this system has become quite saturated during the day. It appears that we need to increase our capacity for data analysis and we are currently investigating possibilities.

4. INSTRUMENTS

4. IPNS INSTRUMENTS

The instrument package at IPNS is shown in Fig. 7. Particular attention has been paid to using the rich epithermal spectrum of neutrons that is present in such a spallation source. For example at 500 meV (λ = 0.4 Å) IPNS has an effective flux ~10 times greater than at the ILL hot source.

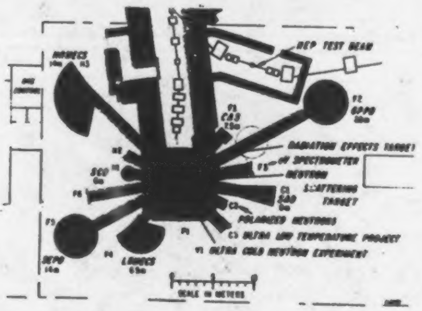


Fig. 7. Experimental Facilities. The proton beam enters the target area from the top of the figure and strikes one of two uranium targets, one for fast neutron irradiation studies (the radiation effects target), and the other for neutron scattering. The latter is surrounded by (hydrogenous) moderating material. The acronyms for the instruments and their general areas of research are given in the text.

The instruments for elastic or total scattering consist of 2 powder diffractometers (SEPD — Special Environment Powder Diffractometer, GPPD — General Purpose Powder Diffractometer) which have excelled at high-resolution work, coupled with the on-line capability of the Rietveld analysis, and also proved useful for amorphous systems. The Single Crystal Diffractometer (SCD) is based on the Laue technique with a position-sensitive two-dimensional (30 × 30 cm) detector designed and built at Argonne (scintillation detector based on the Anger method) and has investigated crystal structures, and various problems involving superlattice or diffuse scattering. The Small Angle Diffractometer (SAD) also includes a position-sensitive detector used to investigate both metallurgical and biological problems. Of particular interest is the attempt to use the epithermal neutrons in resonant small angle scattering on biological molecules.

The two chopper spectrometers (LRMECS — Low-Resolution Medium-Energy Chopper Spectrometer, HRMECS — High-Resolution Medium-Energy Chopper Spectrometer) have proved exceptionally versatile in a variety of problems involving measurements of $S(Q,\omega)$. Experiments on amorphous materials, electronic transitions, and momentum distributions have all made use of the abundant epithermal spectrum to perform measurements up to 300 meV energy transfer at low values of momentum transfer. For inelastic scattering the Crystal Analyzer Spectrometer (CAS) is particularly well suited to examine dispersionless high-energy vibrational modes.

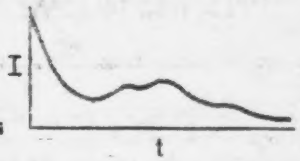
Other so-called "special" experiments include an effort on polarized neutrons, an experiment at ultra-low temperature designed to investigate nuclear ordering in ^{3}He, and a search for the electric dipole moment of the neutron with a pulsed source. A new instrument, an eV spectrometer, is under construction. The first table shows parameters of each instrument and details of special experiments. Also shown is information on allocation of the instruments to users.

The next section is devoted to descriptions of the instruments, with accounts of some experiments performed on them, together with details of the "special" experiments. All personnel involved in work on these instruments are listed at the end of this section.

Specially highlighted throughout this volume is work of particular interest. This includes: High-Energy Electronic Spectroscopy; Scintillation Detectors; Proton Therapy; ^{4}He Momentum Density; and Structural Investigations using Rietveld Analysis.

SPECIAL ENVIRONMENT POWDER DIFFRACTOMETER

The special environment powder diffractometer (SEPD) began operation August 4, 1981, the first day neutrons were produced in the scattering target. The first calibration and exploratory measurements began roughly one week later and the formal user program commenced November 16. Scientists particularly involved with the powder instrument are J. D. Jorgensen, J. Faber, M. H. Mueller, F. J. Rotella, J-E. Jorgensen and R. L. Hitterman.



IPNS EXPERIMENTAL FACILITIES

NEUTRON SCATTERING

Facility (Instrument Scientist)	Assignment	Range		Resolution	
		Wavevector[*] ($Å^{-1}$)	Energy (eV)	Wavevector	Energy
Special Environment Powder Diffractometer (J. D. Jorgensen)	F5	0.5-30	[**]	0.35%	[**]
General Purpose Powder Diffractometer (J. Faber, Jr.)	F2	0.5-100	[**]	0.25%	[**]
Single Crystal Diffractometer (A. J. Schultz)	H1	2-20	[**]	2%	[**]
Small-Angle Scattering Diffractometer (J. E. Epperson[†] and C. Borso[††])	C1	0.001-0.3	[**]	0.004 $Å^{-1}$	[**]
Low-Resolution Medium-Energy Chopper Spectrometer (C-K. Loong)	F4	0.1-30	0-0.6	0.02 K_o	0.05 E_o
High-Resolution Medium-Energy Chopper Spectrometer (D. L. Price)	H3	0.3-9	0-0.4	0.01 K_o	0.02 E_o
Crystal Analyzer Spectrometer (T. O. Brun)	F1	3-16	0.02-0.5	3%	2%

NEUTRON BEAMS FOR SPECIAL EXPERIMENTS

Beam Tube	Current Use	Flight Path Length (m)
F3	eV Spectrometer	10
C2	Polarized Neutron Experiment	10
C3	Solid ^{3}He Project	10
F6	Irradiations	6-20
H2	Irradiations	6-20
V1	Ultracold Neutron Experiment	4

RADIATION EFFECTS

Facility (Instrument Scientist)	Description
Radiation Effects Facility (R. C. Birtcher)	Two vertical (5 cm ID) tubes with flux 1×10^{12} n cm^{-2} s^{-1} and one horizontal (3.8 cm ID) tube with flux 3×10^{11} for energy greater than 0.1 MeV at 8 μA; capabilities for maintaining two samples at liquid helium temperature (4 K) and above.

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[*] Wavevector, $K = 4\pi \sin\theta/\lambda$.

[**] No energy analysis.

[†] Materials Science — 3 m flight path.

[††] Biology — 8 m flight path.

ALLOCATION OF USER INSTRUMENTS

	Number of Experiments								
	SEPD	GPPD	SCD	SAD	LRMECS	HRMECS	CAS	REF	TOTAL
1981									
November	7	5	1	—	—	—	—	—	
December	7	3	1	—	1	—	—	—	
1982									
January	3	2	—	—	1	—	—	3	
February	3	3	1	—	1	—	—	3	
March	7	4	3	—	2	—	—	3	
April/May	10	6	4	—	1	—	3	2	
June	7	3	1	—	2	*	1	4	
July	13	10	4	—	3	2	3	5	
October	—	—	—	—	1	1	—	9	
November	3	1	1	—	1	1	—	3	
December	3	—	1	—	1	1	—	2	
1983									
March	3	4	1	*	1	1	—	10	
April	4	5	3	4	4	2	2	—	
May	6	4	1	3	3	2	1	—	
June	6	4	2	1	2	1	3	—	
July	4	4	1	2	1	2	—	5	
	86	58	25	10	25	13	13	49	279
Experiments Performed by Scientists at ANL:	45	15	5	4	7	1	6	19	102
ANL 6 Visitor	24	25	19	4	10	12	6	17	117
Visitor Only	17	18	1	2	8	—	1	13	60

*Instrument Commissioned.

Instrument tuneup proceeded with no major problems and overall performance agreed with design specifications. Diffraction data on calibration samples indicated that the useful thermal flux scaled as expected from ZING-P, being approximately 2×10^5 n cm^{-2} s^{-1}. Using the original polyethylene moderator the resolution (in backscattering) varied from 0.28% ($\Delta d/d$) at d = 3 Å to 0.57% at d = 0.6 Å.

The SEPD continued to operate routinely with no problems during 1982. During the first year of operation, over 200 data sets were collected, representing 35 separate experiments. The majority of these experiments (19) were proposed by principal investigators outside Argonne; an additional 8 came from Argonne scientists not previously associated with the neutron powder diffraction program.

Normal operation of the SEPD was curtailed during the operation of the liquid methane moderator from September 1982 to February 1983. The cold moderator gave a substantial increase in flux at long wavelengths, but caused broader peaks with a shape which could not be fitted by the resolution function currently used in the Rietveld refinement code. Thus, a room temperature polyethylene moderator was installed during February 1983 and full operation of the powder diffractometers by outside users resumed March 1, 1983. The new polyethylene moderator is poisoned to give about 10% better resolution than the previous one with a slight loss of flux.

Considerable effort has been devoted to determining the sources of sample-dependent background and finding ways to improve the signal-to-noise ratio of the SEPD. It was found that a significant background contribution resulted from high energy neutrons scattered from the sample and then scattered again (possibly several times) from the instrument shielding or sample chamber before being detected. Tests showed that much of this multiple scattering background can be eliminated with correctly placed shielding inside the scattered flight path. New shielding fabricated from boron carbide epoxy was installed during July 1983. A significant improvement in the quality of data, especially at high neutron energies, was achieved. This should be particularly helpful for high Q measurements on amorphous systems.

The present instrument configuration has a total of 120 active detectors in mirror image positions (right and left sides) in groups centered at $2\theta = 150°$, 90°, 60° and single groups at 30° and 14°. This configuration allows measurement of d spacings from 0.1 Å to 25 Å ($Q = 0.2 - 60$ Å^{-1}).

Counting times vary greatly with sample size and the complexity of the structure, and have ranged from 6 hours for small cubic cells ($V \sim 180$ Å^3) and glass samples to 2 or 3 days for weak, large d, magnetic peaks in a complex monoclinic system and for samples in the pressure cell. Twelve to 24 h is typical for most samples.

An effort has been made to offer more special environment equipment to the users. A simple furnace allows heating to 300°C. A higher temperature furnace has been operated to about 950°C. A closed-cycle Displex refrigerator has been operating since mid-December 1982 and provides 12-300 K with no additional peaks or incoherent background in the data. A supported, piston-in-cylinder pressure cell has been used for two experiments in the 25-30 kbar range and is now being scheduled for experiments by outside users.

Some unique instrument capabilities have been observed. The SEPD appears to be an unusually good glass/amorphous diffractometer because of its low background extending to high energies. Recent measurements exhibit usable data at momentum transfers above 40 Å^{-1}. D. Price has written analysis codes which reduce amorphous data to S(Q) and G(r) with attenuation, multiple scattering and inelastic corrections.

Total cross-section measurements at high energy ($\sim$400 meV) have been made to help verify sample composition. This has been useful in measuring hydrogen content in PbO_2 from battery electrodes and in monitoring the in situ thermal decomposition of $CaSO_4 \cdot 2D_2O$ to $CaSO_4 \cdot 0.5D_2O$. Accuracy of 5% or better seems possible.

The low angle, electronically focused detectors allow unusually good resolution and intensity at large d spacings. G. Felcher and R. Wappling of the University of Uppsala solved the magnetic structure of monoclinic FeGe by indexing magnetic peaks in the 2-8 Å range. (The resolution is 1% out to 8 Å at 57°.)

The first high pressure diffraction experiments were performed on the SEPD in the second year using a pressure cell which was previously used at ANL's CP-5 reactor. The sample is sealed in a teflon tube which is placed in a sintered alumina cylinder supported by a series of steel building rings. Windows in the steel allow neutron transmission at selected angles. The first high pressure experiments to be performed were bismuth III at 30 kilobars by T. G. Worlton and J. D. Jorgensen, and D_2O ice VII at 24 kilobars by J. D. Jorgensen, T. G. Worlton, and M. Grimsditch. Effective sample volume in the pressure cell is about 0.2 cm^3. At a scattering angle of 90° with a proper choice of active detectors, it is possible to obtain data which is free from any impurity peaks due to the pressure cell.

Typical data collection times for these two experiments were about two days at each pressure.

The first liquid diffraction data to be taken on the SEPD was a study of $LiA\ell$ near its melting point (697°C) by J. R. D. Copley (McMaster Univ.), W. S. Howells (Rutherford), D. L. Price, S. Susman, and T. O. Brun. Data collection times of only a few minutes were sufficient to identify phases and locate the melting point (Fig. 8).

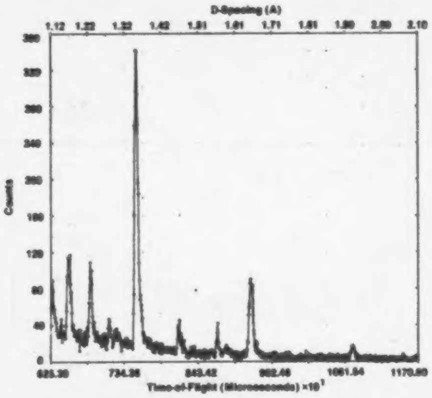


Fig. 8. Section of Raw Data for $LiA\ell$ Just Below Its Melting Point, 697°C. Bragg peaks are from $LiA\ell$ Zintl phase and a tantalum sample can. Data collection time was 15 min.

In another unique experiment by L. Guttman, G. P. Felcher, S. K. Sinha, and G. E. Fish (Allied Corp.) a sample of $Fe_{1-x}B_x$ amorphous alloy was studied in an 1100 Oe magnetic field. Data for the field perpendicular and parallel to the scattering vector were collected simultaneously in the opposing 90° detector banks by appropriate orientation of the magnet.

Future plans include the construction of two more pressure cells. (1) A gas pressure cell for the range 0-8 kilobars which will offer a larger sample volume, precise pressure control, and the ability to cool with a cryostat. (2) A clamp-type, piston-in-cylinder cell which will reach the 20-30 kilobar range and can be mounted in a cryostat for low-temperature, high-pressure measurements. This equipment should become operational within 1984.

GENERAL PURPOSE POWDER DIFFRACTOMETER

The general purpose powder diffractometer (GPPD) has been operating in the high-resolution configuration (source-to-sample distance = 20 m) since August 1981. Significant reductions in sample-dependent background were obtained with borated polyethylene shielding installed in the scattered flight path of the GPPD. Coarse detector bank collimators installed in the spring of 1983 reduced the sample dependent background by ~50%. Other shielding tests on the chopper spectrometers and the SEPD have confirmed our results. New boron carbide shielding elements are currently under fabrication which should be more effective at short wavelengths.

The samples involved included ceramics, hydrides, metal alloys, metallic glasses, oxides and organic materials. Successful Rietveld profile refinement analyses on monoclinic ABO_4 compounds (Aldred and Faber) required 38 adjustable parameters to fully describe the structural detail, including anisotropic thermal vibration. The unit cell volume for these compounds is approximately 320 $\AA^3$. Excellent resolution, $\Delta Q/Q \sim 0.0025$ at $2\theta = 152°$ was an important factor in our ability to resolve the structural detail. Experiments are routinely carried out in the range $0.6 \leq Q \leq 30$ $\AA^{-1}$. To demonstrate the dynamic range of Q available, experiments were carried out on $TbFe_4A\ell_8$ (Shaked from Negev, Israel, Faber and Hitterman) to measure satellite reflections ($10 \leq T \leq 80$ K) at small Q. At large Q, the three lowest energy nuclear resonances for Tb (E = 3.3, 5 and 12 eV) were also observed. Complex crystal structures (unit cell volumes ~ 3500 $\AA^3$ and monoclinic cell symmetry) have been attempted (Aldred and Faber). Successful experiments were completed on deuterated tooth enamel (Young and Suitch, Georgia Tech.). Experiments were routinely carried out in the range $10 \leq T \leq 300$ K with a Displex refrigerator, and up to 300°C with a small furnace. A number of experiments were completed on amorphous materials (e.g., Wagner, UCLA; also Nagel and Busse, Univ. of Chicago). In this case, $0.5 \leq Q \leq 30$ $\AA^{-1}$ were measured.

A demonstration of GPPD high resolution capabilities on complex crystal structures is illustrated in Fig. 9, where we show only the small d-space region of data collected on chromium molybdate by P. Battle, T. Cheetham, and J. Faber. Over 100 adjustable parameters and ~4000 independent hkℓ's are required to fit the range $1.13 \leq d \leq 3.9$ Å, which corresponds to $2.1 \leq Q \leq 8.3$ Å^{-1} at $2\theta = 90°$. The unit cell volume $V_c = 2100$ Å^3 with 34 atoms in the unit cell. Considerable input based on chemical information and anticipated bonding arguments is required to refine the structural model at this level of complexity.

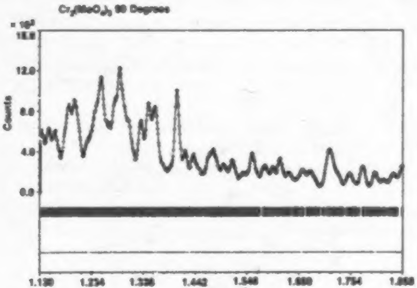


Fig. 9. Neutron Diffraction Study of Chromium Molybdate Using the GPPD. The + signs are experimental data after background subtraction. The solid curve is the calculated pattern. The vertical ticks show the positions of the independent hkℓ's in d-spacing. The differences between the data and calculation are plotted in the lower portion of the figure.

Several experiments (MacEwen, CRNL, Faber and Turner) have been successfully carried out to measure residual grain interaction stresses in deformed, polycrystalline, hcp Zircaloy-2 alloys. The results are illustrated in Fig. 10, where we can see that a plastic tensile strain (~3%) causes the (1010) prism reflection to shift to larger interatomic planar spacings, while the (0002) basal reflection shifts to lower spacing. A compressive deformation reverses the direction of the peak shifts, with prism and basal planes being left in residual compression and tension, respectively. The magnitude and sign of the residual stresses, which result from the interaction among different grains in the deforming polycrystalline specimen, are consistent with the texture and anisotropic yield surface of zircaloy. Successful experiments were also carried out on deformed WC cermets (Krawitz, Univ. of Missouri, and Faber), where residual stresses in both the WC parent phase and Co-Ni binder phase have been detected. We estimate that residual stresses of order 10^{-5} can be routinely detected using the high resolution configuration on the GPPD.

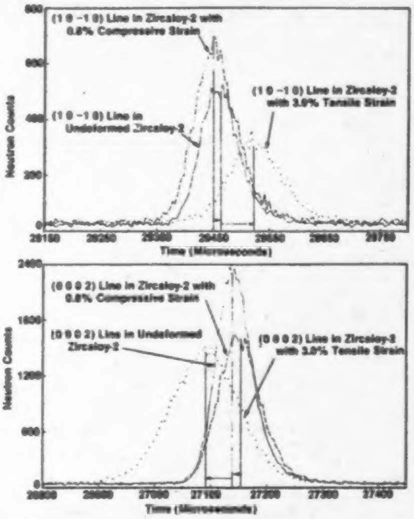


Fig. 10. Line Profiles Taken on GPPD for Two Reflections of hcp Zircaloy-2 Rods Under Different Conditions.

Nearly 50% of the experimental time on the GPPD required the use of ancillary equipment. A Mark II vacuum furnace was successfully tested and used for polycrystalline and high resolution single-crystal studies ($400 \leq T \leq 775$ K) by S. R. MacEwen, CRNL and J. Faber. Both a_0 and c_0 in hcp single crystal zircaloy were measured simultaneously as a function of T by judicious choice of crystal orientation.

STRUCTURAL INVESTIGATIONS USING RIETVELD ANALYSIS

Spallation neutron sources are particulary well suited for structural investigations of polycrystalline material because of the excellent resolution available. The favorable conditions arise because the intrinsic pulse width from the source is a function of energy, being shorter for the higher-energy neutrons, and this is matched to the better time resolution required for the faster neutrons to preserve a constant $\Delta Q/Q$ in the expression for resolution. An additional (obvious) advantage is that we have replaced angular resolution, which is a feature of continuous x-ray or neutron sources, with time-of-flight resolution. A feature of the diffractometers at IPNS is the constant resolution over a wide range of momentum transfer.

In structural investigations another key factor is the ability to refine **all** the data against a model. This "Rietveld" technique — named after the Dutch crystallographer who first developed it — fits all the data points and has greatly enhanced the information content of powder diffraction from both continuous and pulsed sources.

An example of such a study is that on the Chevrel ternary phases MMo_6S_8, where M = Sn, Pb or various rare earths. Interest in these materials stems from the fact that they exhibit interesting superconducting and, provided M = rare earth element, magnetic properties. However, many investigators have reported a wide variety of T_c and lattice parameter values that show a strong need for better material characterization. Hinks, Jorgensen, and Li of ANL set out to investigate this by synthesizing a series of these compounds with varying oxygen impurity levels. Figure A shows the strong correlation between T_c and the c/a ratio (with a ≅ constant and c decreasing) as a function of oxygen defect concentration. Neutron powder-diffraction patterns were then taken of a series of these samples in an attempt to locate the additional small amount of oxygen. This is a difficult task given the essential defect nature of the oxygen site, but a series of internal consistency checks may be applied to the refinement which give confidence in the solution.

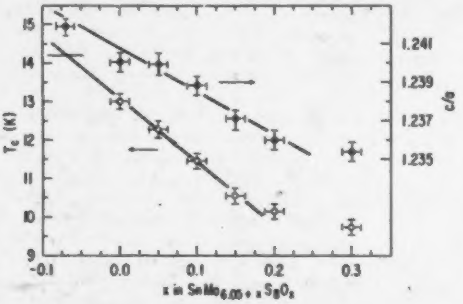


Fig. A. Variation of T_c and c/a (hexagonal lattice-constant ratio) with Added Oxygen in the Sn-Mo-S-O System.

The local structure in the region of an oxygen defect is shown in Fig. B. In the normal $SnMo_6S_8$ structure, Sn is located at the origin, halfway between the two S2 atoms on the $\bar{3}$-axis and is not strongly bonded to any of its sulfur neighbors. In unit cells where an oxygen atom replaces one of the S2 atoms, the Sn atom moves off the origin and forms a short Sn-O bond. From these results we can say that the Mo-Mo and Mo-S lengths in the Mo_6S_8 cluster are not dramatically perturbed

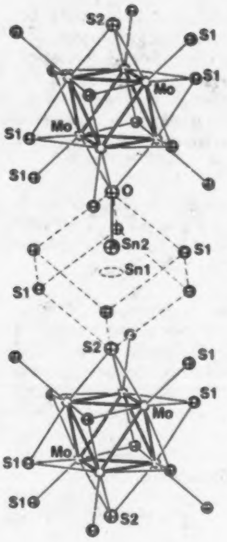


Fig. 8. Local Structure in the Region of an Oxygen Defect.

by the oxygen defect. Furthermore, the intercluster distances (both Mo-Mo and Mo-Si) remain constant. Locally, the structure collapses towards the oxygen impurity. The short bond length might suggest a change in the charge state of Sn resulting in additional charge transfer to the Mo_6S_8 cluster, thus changing the density of states at the Fermi energy and depressing T_c. However, the constancy of the Mo-Mo bonds lengths indicates this is not the case. Changes in either the phonon spectrum or band structure are other possible explanations for the depression of T_c. Neutron diffraction has therefore been responsible for bringing a more scientific perspective to the characterization of defects in these interesting materials.

ANALYSIS OF NEUTRON POWDER DIFFRACTION DATA

FORTRAN software for the display and analysis of time-of-flight (TOF) neutron powder data from the general purpose and special environment powder diffractometers is operational on our IPNS-dedicated VAX-11/780 computer. At the heart of this software package are the routines TOFPRP and FOFLS (written by R. B. von Dreele of Arizona State University and used extensively at Argonne over the past 4 years) which perform full-matrix least-squares refinement of crystal structure and peak shape parameters (Rietveld analysis) based on powder data. Programs to determine Bragg reflections for a given structure, to calculate Fourier syntheses, to calculate distances, angles and associated standard deviations from refined structures and to illustrate the atomic arrangements of a given structure have been adapted for use in this package. In addition, codes have been written locally to extract and display raw powder data at a specified scattering angle versus TOF and d-spacing, to generate publication quality lists of raw data versus TOF and d-spacing, to indicate the instrumental parameters (i.e., calibration, resolution and incident neutron spectrum) for the standard detector arrangements of the two IPNS powder diffractometers, to update starting least-squares variables with their refined values for use in subsequent refinements and to plot the observed and calculated profile comparatively for publication.

A recent addition to our Rietveld analysis package is a program, developed at Argonne in collaboration with T. M. Sabine of the New South Wales Institute of Technology, Australia, that simulates a TOF neutron powder diffraction spectrum from a known model and calibration, resolution and incident spectral characteristics of a given instrument and scattering angle. Since statistical scatter is built into the simulated spectrum, it resembles raw TOF powder data, and therefore it can be used with the Rietveld refinement codes. This simulation routine has been utilized in assessing the feasibility of possible powder diffraction experiments for IPNS, in testing the physical nature of existing and new functional forms for variables in the refinement scheme, in aiding in the solution of partially known or unknown crystal structures, and in qualitatively and quantitatively identifying the components of mixed-phase samples.

Most of the Rietveld analysis routines mentioned above are also supported on Argonne's IBM-370 computing system. A user's guide to the Rietveld analysis of powder data at IPNS, which describes the form of the input to all the aforementioned programs, is available to all IPNS powder diffraction users. Generally, users who have stayed an extra day or two after data collection have been able to leave with nearly complete Rietveld refinements.

Below is a list of users to whom copies of the VAX/VMS Fortran programs in the IPNS Rietveld data analysis package were exported:

The majority of these users have had little difficulty in either using the exported routines on their "own" VAX or adapting the codes for use on non-VAX systems.

Users at Northwestern University, University of Illinois at Chicago and University of Louisville, Kentucky, have taken powder diffraction data at IPNS and analyzed the data "at home" by dialing up the IPNS VAX.

User	Affiliation
T. M. Sabine	New South Wales Institute of Technology
W. H. Baur	University of Illinois at Chicago
C. Saw	ORNL — currently ANL
R. A. Young	Georgia Institute of Technology
R. G. Teller	SOHIO
J. Newsam	Exxon
J. C. Boyce	Xerox
J. Parise/G. A. Jones/R. Harlow	E. I. du Pont
G. G. Christoph	Ohio State University/3M Company — currently LANL
M. W. Johnson	RAL
R. O. Simmons/P. Sokol	University of Illinois Champaign/Urbana
D. E. Cox	BNL
R. B. von Dreele	Arizona State University
G. A. Jeffery	University of Pittsburgh
P. Rudolf	University of Texas at Austin
J. Schefer	Institut fur Reaktortechnik, ETH

SINGLE CRYSTAL DIFFRACTOMETER

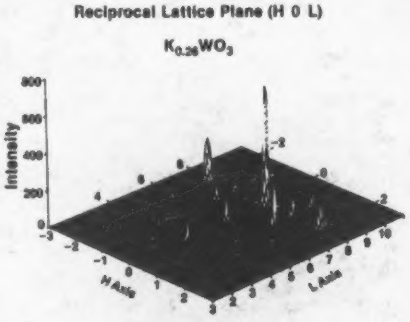
Scientists involved with work on this diffractometer are A. J. Schultz, P. C. W. Leung, R. G. Teller, M. A. Beno, and J. M. Williams. The first experiment performed on the Single Crystal Diffractometer (SCD) was to collect data at 25 K and determine the crystal and molecular structure of methylcyclohexenylmanganese tricarbonyl, $Mn(CO)_3(C_6H_8CH_3)$. The crystal preparation and the room temperature x-ray structure were accomplished by M. Brookhart, W. Lamanna, and M. Beth Humphrey of the University of North Carolina. The low-temperature neutron structure was solved independently by direct method — to our knowledge, the first such case with time-of-flight data. The structure contains an unusual 3-center, 2-electron, C-H-Mn interaction, with C-H = 1.19(1) Å and Mn-H = 1.84(1) Å. The data were obtained with the new 30 × 30 cm position-sensitive ^{6}Li-glass scintillation detector developed by M. Strauss and R. Brenner of the Electronics Division.

In 1982, M. Beno led the effort to design and build a new mount for the closed-cycle Displex helium refrigerator (10-300 K). The refrigerator is now completely supported by the phi base on one side of the chi circle. The mount permits translational adjustments in three directions and preliminary tests indicate the sample will remain centered to within 0.1 mm or less. Since the vacuum shroud does not span the chi circle to provide additional support, a crystal can be optically aligned on the diffractometer before attaching the aluminum vacuum enclosure. Furthermore, since the enclosure does not extend very far beyond the center of the circle, there is less interference with shielding and a much larger region of reciprocal space is accessible.

We have also completed the structure of the coordination complex $[Re(CO)_4(CH_3CO)_2]H$ in collaboration with C. Lukehart of Vanderbilt University. The molecule contains an interesting intramolecular O-H-O hydrogen bond which exhibits an unusual PMR chemical shift. This is the second organometallic molecular structure that has been completed with SCD data.

A number of improvements were made on the SCD in 1983. During the shutdown in January and February, R. Brenner and M. Strauss (Electronics Division) took apart and re-assembled the position-sensitive area detector to reduce the distortion where the four pieces of ^{6}Li scintillation glass are joined and to improve the light coupling between the scintillation glass and photomultipliers. Another improvement is the use of variable time channel widths rather than constant channel widths as in the past. This new option permits data in different wavelength regions to be histogrammed with approximately the same resolution. G. Anderson (Northern Illinois University) has assisted us in writing some programs which can plot intensities for points along any reciprocal lattice vector or on a plane which intersects or passes through a histogram. These programs are particularly useful for determining symmetry absences and for characterizing superlattice scattering.

One of the applications for this graphics software is shown in Fig. 11 for data from a crystal of $K_{0.26}WO_3$.


Reciprocal Lattice Plane (H 0 L)

$K_{0.26}WO_3$

Fig. 11. Neutron Diffraction Data from a Crystal of $K_{0.26}WO_3$.

The x-ray structure was reported to have space group $P6_3/mcm$, for which the $h0\bar{h}\ell$ data, $\ell = 2n + 1$, are absent. As is clearly observable in the figure, these peaks are not absent in the neutron data. In addition, the data exhibit satellite peaks which are presently being analyzed in terms of a superlattice structure. H. B. Krause of Northern Illinois University is the principal investigator for this experiment.

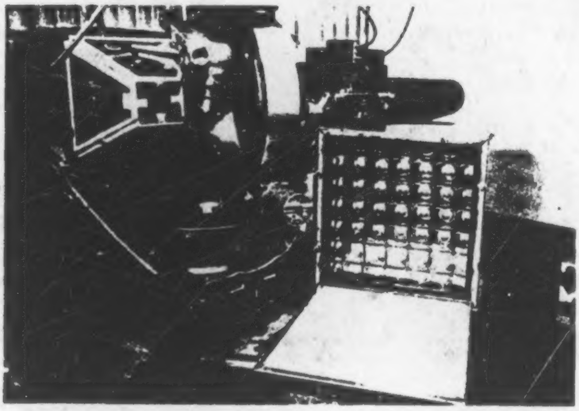
2-DIMENSIONAL NEUTRON-POSITION SCINTILLATION DETECTORS

Pulsed neutron sources produce high instantaneous flux with a broad energy spectrum where a significant fraction of the neutrons is in the epithermal range. A suitable neutron detector should therefore have high count rate capability and high detection efficiency extending to epithermal energies. A 2-dimensional position-sensitive scintillation detector which meets these requirements was developed by M. Strauss and R. Brenner of the ANL Electronics Division.

The detector shown in the figure, is comprised of an array of photomultiplier tubes (PMT's) coupled via a disperser to a thin ^{6}Li-glass scintillator. Neutrons absorbed in the glass produce scintillation flashes which give rise to signals in the surrounding PMT's. These are processed by analog circuits that calculate the X and Y centroids of the neutron position of interaction. The coordinates are digitized and stored in a computer along with the corresponding neutron time-of-flight. X-Y distribution maps are generated for each neutron energy of interest. A FWHM of less than 3 mm has been achieved. The detector can be made round or square and can even have a neutron through-hole in the center of the scintillator. A 30 × 30 cm^2 detector consisting of 49 square PMT's (51 × 51 mm^2) is incorporated in the single crystal diffractometer at IPNS.

Compared with the gas proportional counter, this new scintillation detector has higher epithermal neutron detection efficiency, considerably higher instantaneous count-rate capability, and negligible parallax error. Yet its cost of fabrication is less than half.

Because of the detector versatility, performance, and potential, it has been drawing worldwide attention. Similar detectors are now being developed in the U S and several other countries. A high resolution detector (FWHM = 1-1.5 mm) is being developed at Argonne for ILL.



The Figure shows the Goniometer of the Single Crystal Diffractometer (center) with the shielding of the PSD on the Left. The PSD itself has been placed on the right of the picture for ease of viewing. The scintillator screen (bottom right) has been removed from the detector to expose the square array of photomultiplier tubes.

H. Horiuchi (Osaka University, Japan) designed and constructed a furnace (Fig. 12) which he used to collect high temperature data on a crystal of yttrium-stabilized zirconium oxide (YSZ), which conducts oxygen ions at elevated temperatures. The furnace is stationary during data collection and is simply suspended in the center of the diffractometer with openings in the outer alumina container for the incident and unscattered beam and for the neutrons scattered by the crystal toward the detector. The crystal is mounted on a silica glass rod which passes through a slit in the furnace and permits the crystal to be rotated more than 90° in chi and a full 360° in phi. Data on a crystal of YSZ were measured at room temperature, at 760° with and without a potential of 7.8 volts placed across the [100] and [$\bar{1}$00] faces of the crystal. The goal is to characterize any structural differences which may exist between the low-temperature nonconducting state and the high-temperature conducting state.

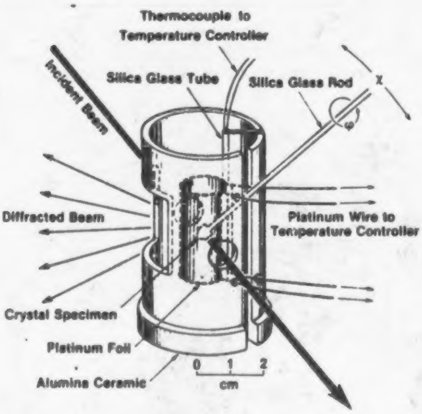


Fig. 12. A Drawing of the Furnace Used on the SCD. The volume between the platinum foil and the alumina cylinder is filled with quartz glass wool to provide thermal insulation.

In the future, we plan to test a new vacuum shroud for the Displex helium refrigerator. The new apparatus was designed by R. Kleb to reduce the amount of scattering from the aluminum shroud which can reach the detector. This should significantly reduce the background and permit improved analysis of diffuse scattering and superlattice peaks. We are also investigating methods for improving the accuracy of the detector encoding. In addition, we are investigating different algorithms for integrating peaks.

SMALL ANGLE DIFFRACTOMETER

The background problems that plagued the early efforts with this instrument have been reduced to the point where the ratio of the integrated flux on sample to the empty camera background is now about 6×10^6. This was accomplished, principally, by replacing the continuous tapered steel collimators with a series of apertures, the final two consisting of enriched ^{10}B.

With the spectrum of neutrons available from the room temperature polyethylene moderator and the present collimation system, the momentum transfer was restricted to the range $0.02 \leq Q \leq 0.35$ Å^{-1}. However, the 80 K moderator installed during the August-September 1983 shutdown will extend this range down to 0.008 Å^{-1}. Also during this shutdown period, a new data collect computer was installed (PDP-11/24) which permits display during data collection. A furnace capable of operating up to 1000°C is now available.

Software is operational to permit routine correction of the scattering data for detector sensitivity, wavelength-dependent absorption, background, and for performing radial averages. A battery of options is then available in an interactive code for analyzing the reduced data in terms of the relevant materials parameters. Data analysis software is also available for biological applications for determining radial distribution functions and other parameters via the indirect transformation methods of Moore and Glatter.

Figure 13 shows a profile measured for an Aℓ-5 at% Zn alloy; the peak is a well documented feature for this system and, along with the effective Guinier radius, is in good agreement with previous

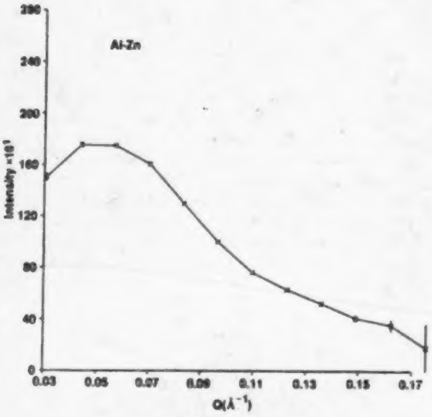


Fig. 13. Intensity Versus Q for an Al-5 at% Zn Alloy. The peak is normally associated with interparticle interference.

measurements. The work on materials problems and glasses is being undertaken by E. Epperson and his collaborators. Figure 14 illustrates a series of radial distribution functions obtained from the scattering profiles from a series of rhodopsin samples by varying the D_2O and sucrose concentration of the solvent. The data analysis was performed using the algorithms developed by P. Moore (Yale). The results are being used by C. Borso and his collaborators in the Biology Division to clarify the discrepancy between the x-ray and neutron structure previously determined for the rhodopsin-detergent complex. Structural information is needed to help understand the function of this important protein in the visual process, since it is the primary photoreceptor in a chain of photochemical events initiated by the transduction of light.

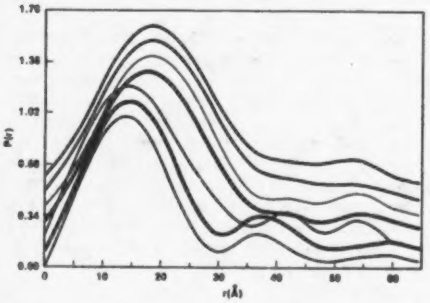


Fig. 14. Radial Distribution Functions for the Rhodopsin-Detergent Complex with Varying Sucrose Concentration in 100% D_2O.

D. Worcester and L. Braganza (ILL) carried out an investigation on rat sciatic nerve myelin membranes to study the chemical and physical properties which cause the membranes to adhere, and thus maintain the myelin sheath necessary for nerve signaling. It was found that increasing the hydrostatic pressure caused the membranes to separate measurably, and this was attributed to increasing membrane surface charge. Figure 15 shows two Bragg peaks from myelin sheath membranes, the spacing between these peaks being related to the membrane spacing of 174 Å. This work has suggested new ideas about how the membranes behave in pathological conditions, such as multiple sclerosis.

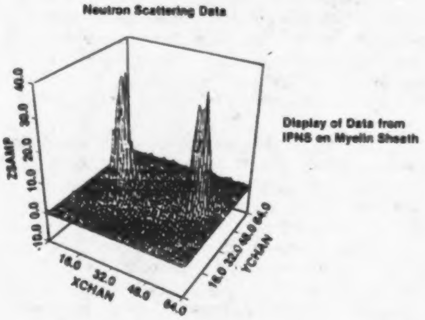


Fig. 15. Bragg Peaks from a d-Spacing of 87 Å as Registered on the Small-Angle Diffractometer from a Sample of Myelin Sheath from a Rat Sciatic Nerve.

CHOPPER SPECTROMETERS

The low-resolution (LRMECS) and high-resolution (HRMECS) medium-energy chopper spectrometers are operating routinely for scheduled experiments. To accommodate experiments requiring a large range of incident neutron energies and different resolutions, three new choppers were built in 1983, two of which have a 3 in-wide by 4 in-high slit package matching the full beam size of HRMECS. Together with the existing two choppers, choices of incident energy from ~30 meV up to 1 eV are easily arranged. All choppers are operational with measured duty cycles of over 99%.

During 1983, improvements were made in beam monitoring, and some important shielding improvements, to reduce fast neutron background, were also added. The albedos (reflection coefficients) of several materials which might be used for shielding inside spectrometers were measured on LRMECS at 800 meV. Among the more practical materials, we found that epoxy-bonded (≤10% epoxy) natural B_4C has a low albedo. Boral plate is nearly as good, with BN somewhat poorer. Consequently 1/2 in-thick epoxy-bonded B_4C plates were placed behind the detectors in HRMECS to eliminate reflection of neutrons from the back walls of the spectrometer, which had been previously observed. In addition, boral "baffles" were attached to the floor, ceiling and walls of the flight path to prevent reflection of neutrons into the detectors. Spectacular gains in signal-to-noise ratios were achieved as a result. Similar improvements are now completed at LRMECS.

By May 1982, the high-intensity, low-resolution instrument (LRMECS) had been operating for several months and experiments approved by the Program Committee were underway. Measurements of the vibrational densities of states of amorphous SiO_2 and amorphous P have been completed and demonstrate the capability of the chopper spectrometers at IPNS to contribute unique information toward the understanding of the structure and dynamics of amorphous solids. As an example we show the measured scattering function S(Q,E) for SiO_2, a typical tetrahedrally coordinated network glass much studied by other techniques.

We chose the incident neutron energy E_0 = 220 meV with the sample at 20 K to reduce multiphonon scattering. Figure 16 shows the result of measurement after preliminary corrections. Measurements as complete as those shown in Fig. 16 are impossible at reactor sources because beam intensities fall off sharply for energies above ~100 meV. The "elastic" structure factor derived from the data (suppressed in the figure) is in good agreement with earlier measurements and shows the expected fall-off at high momentum transfer due to the effects of thermal vibrations.

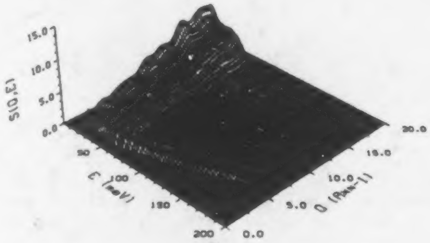


Fig. 16. Scattering Function S(Q,E) for SiO_2. Incident beam energy 220 meV, sample temperature 20 K.

The inelastic structure factors (S(Q,E) at constant E's) show interference effects related to the nature of the normal-mode displacements of this character. These effects are being calculated by L. Guttman with a computer model. The density of states function derived from the data (by averaging over a wide Q-range, $5 < Q < 12$ $Å^{-1}$) is generally in excellent agreement with earlier measurements and model calculations, while the data have good statistical accuracy over their entire range. Further, the splitting of the highest frequency peak is clearly revealed - this has not been the case in earlier neutron measurements.

HRMECS came into operation in May 1982 and has performed according to specifications. Thanks to the efforts of G. Ostrowski, and I. Jung of the Electronics

DETERMINATIONS OF MOMENTUM DISTRIBUTIONS BY DEEP INELASTIC SCATTERING

The isotopes of solid helium (^{4}He and ^{3}He) are extreme examples of a quantum solid in which quantum-mechanical uncertainties in the atomic positions are a large fraction of the interatomic spacing. In order to calculate the physical properties of such a system it is necessary to know the wavefunction in the ground state. This, however, is a formidable problem since the way in which the wavefunctions of individual particles are combined in the wavefunction of the entire system depends critically on correlations between the positions of nearby particles. Although considerable progress has been made in theoretical estimates of these correlations, especially by Green's-Function Monte Carlo methods, many uncertainties remain.

Inelastic neutron scattering offers a way of measuring the wavefunction in the ground state through the momentum distribution $n(\underset{\sim}{p})$, which is essentially the Fourier transform of the square absolute value of the wavefunction. If the scattering function $S(\underset{\sim}{Q},E)$ is measured as a function of energy transfer E at sufficiently high wavevectors $\underset{\sim}{Q}$, the scattering can be treated as a collection of scattering events involving isolated atoms of mass M and the scattering function can then be simply written in the form of the "impulse approximation"

$$S(\underset{\sim}{Q},E) = \int n(\underset{\sim}{p})\,\delta\left(E - \frac{\hbar^2 Q^2}{2M} - \hbar^2 \frac{\underset{\sim}{Q}\underset{\sim}{p}}{M}\right) d^3\underset{\sim}{p}. \qquad (1)$$

Measured at a certain value of $\underset{\sim}{Q}$, this function represents a scattering intensity centered at the recoil energy $E_R = \hbar^2 Q^2/2M$ with a shape which reflects the momentum distribution $n(\underset{\sim}{p})$. The impulse approximation is expected to be valid for recoil energies of >100 meV, implying wavevectors $Q > 14$ Å^{-1}.

The epithermal beams from pulsed sources are ideal for such measurements. When the spectrometer is operated at an incident energy of 500 meV, the wavevector Q for an experiment of this kind ranges from 12 to 22.5 Å^{-1} for scattering angles between 48° and 115°, corresponding to recoil energies between 77 and 264 meV. In the first of a series of collaborative experiments by the Low-Temperature Physics Group at the University of Illinois and the Neutron Scattering Group at Argonne, measurements were carried out on hcp ^{4}He at two pressures corresponding to molar volumes $V_m = 18.2$ and 19.5 cm^3. Liquid ^{4}He at $V_m = 18.2$ cm^3 was also measured as a reference point.

A typical experimental curve of the data obtained at one of the eight detector groups is shown in Fig. A. The scattering measured from the empty aluminum cell has been subtracted; this is in any case very small, except for energy transfers near zero, because of the large mass of Al compared with He. The solid curve represents the least-squares fit of a Gaussian curve to the experimental data.

Figure B shows the mean energies of the fitted experimental curves as a function of Q^2. In the recoil approximation, peaks are expected at the recoil energy $E_R = \hbar^2 Q^2/2M$, represented by the straight line in Fig. B. The points lie on the expected line for the larger Q values, but a positive deviation becomes apparent at lower Q; this may represent a departure from the recoil approximation analogous to the "Compton defect" found in x-ray scattering from electrons. The magnitude of the discrepancy (a few meV) is consistent with the effective depth of the potential well in which individual helium atoms are constrained in the solid.

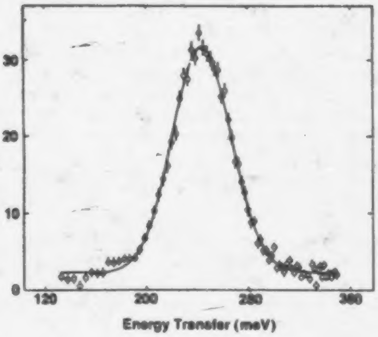


Fig. A. The Measured Scattering Function for the 19.5 cm^3 mol^{-1} Sample at a Scattering Angle of 105.9°. The statistical error bars are shown together with a least-squares fit to the Gaussian form.

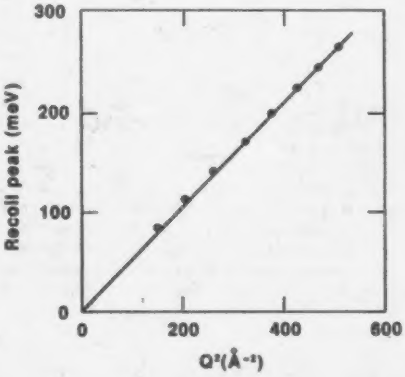


Fig. B. The Peak Positions Fit to S(φ,E) Together With the Straight Line Calculated in the Recoil Approximation. The error in the fitted values is given by the size of the points.

In summary, the momentum distribution n(p) of hcp ^{4}He has been measured directly for the first time using the Chopper Spectrometer at IPNS. The results are consistent with a simplified treatment of the theory and are close to, but not exactly in agreement with, recent computer calculations. The instrumentation appears excellently suited for measurements of this kind in quantum systems and further measurements to investigate the effects of anisotropy, crystal phase, temperature, and pressure are in progress.

HIGH-ENERGY ELECTRONIC SPECTROSCOPY

The neutron interacts with the unpaired electrons around the nucleus because the neutron possesses a magnetic moment. This interaction allows us to obtain unique information about the configuration and dynamics of "magnetic electrons" in condensed matter — information that cannot be obtained by any other technique. The present reactor sources are able to make inelastic scattering measurements up to about 100 meV and it is the extension of this up to higher energies that is a particular challenge for pulsed sources. The problem is a difficult one, primarily because of the form of the neutron-magnetic interaction. Since the electrons have a spatial extent comparable with the wavelength of the neutron (~1 Å) the scattering intensity falls rapidly as a function of momentum transfer, Q. This is illustrated in the figure by plotting the form factor, which appears as the square in the expression for intensity, as a function of Q. This function determines that neutron experiments to search for magnetic interactions must take place with $Q \lesssim 5$ $Å^{-1}$. We then require large energy transfers ΔE at small Q. This immediately poses the well known kinematic restriction, derived from the need to preserve both energy and momentum in the scattering process. To illustrate this, we plot in Fig. A the Q, ΔE space available with an incoming incident neutron energy of 800 meV, which is about the limit with the present choppers at IPNS.

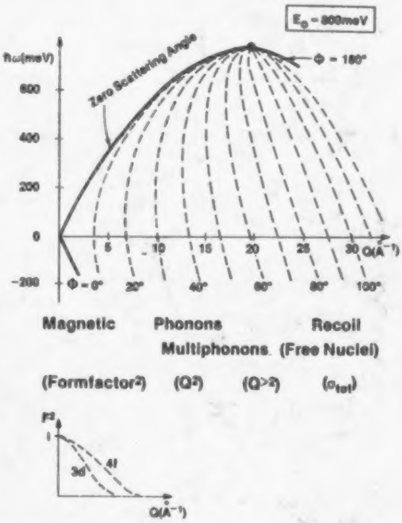


Fig. A. Available Q,ΔE space, with 800 meV incident Neutron Beam.

Despite these difficulties electronic spectroscopy is being performed by a number of groups at IPNS. In Fig. B we show the crystal-field transition observed at 130 meV in PrO_2 by S. Kern (Colorado State Univ.) and his coworkers. This tells us the overall splitting of the ground-state J multiplet in this material and hence the strength of the electrostatic interaction on the magnetic $4f^1$ electron around the Pr nucleus. Similar experiments have been done on UO_2 and are planned on other materials containing f electrons.

In Fig. C we show a slightly different type of measurement, this time done in a single-crystal, of the collective spin-wave in the element Fe, as reported by J. Lynn (Univ. of Maryland), and C-K. Loong (ANL) and their collaborators. Because of the importance of understanding the so-called spin waves (collective excitations of the unpaired electron spins) of iron, nickel, and chromium in the theory of magnetism much effort has been expended on these measurements in the past. The sample is a 23-gram single crystal of pure iron, measured at 10 K. So far, the team has observed the magnetic scattering around the (110) reciprocal lattice point using neutrons of incident energies of 200, 300, and 350 meV. Spin waves at energy transfers in the range 40-150 meV are found to be consistent with an isotropic spin-wave dispersion relation (Fig. C). Successful connection to the previously measured lower-frequency part of the dispersion curve and extension of the data to 150 meV lead us to believe that it is possible to extend these measurements to the detection of optical spin waves and the investigation of the disappearance of spin waves into the Stoner continuum at high wavevectors in both iron and nickel.

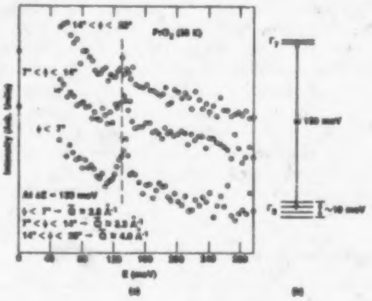


Fig. B. (a) Neutron intensity as a function of energy transfer for three different groups of detectors. The crystal-field transition at 130 ± 5 meV is readily identified. (b) Schematic of the $\Gamma_8 - \Gamma_7$ splitting of the $J = 5/2$ multiplet. The degeneracy of the Γ_8 ground state is lifted by a dynamic John-Teller effect and, in the ordered state, by the exchange field. The neutron excitation corresponds to the total cross-section between all states Γ_8 to both Γ_7 doublet states.

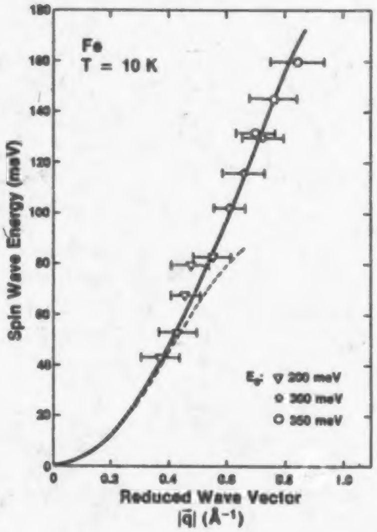


Fig. C. Spin-wave spectrum of pure iron at 10 K assuming an isotropic spin-wave dispersion relation. Incident neutron energies of 200, 300 and 350 meV have been used to measure the magnetic excitations from 40 to 160 meV. The full curve shows the results of fitting the dispersion relation to the experimental data in which D and β were found to be approximately 307 and 0.32 meV Å^2. The dashed curve is calculated using D = 325 meV Å^2 and β = 0.9 meV Å^2 and is that derived from earlier measurements up to 100 meV.

Division, the multichopper phasing system now works excellently and over Summer 1982 three instruments (HRMECS, LRMECS and the ^{3}He experiment) were run simultaneously synchronized with the accelerator. Running machines simultaneously (and possibly choppers on other experiments as well) presented a more complex phasing problem since only one chopper can be used to trigger accelerator extraction. Nevertheless, simulation tests run during April with two choppers controlled by a fixed-frequency oscillator successfully demonstrated that two choppers can be maintained in acceptable phase relationship with the accelerator. At present 94 detectors are in operation covering the range of scattering angle from 4 to 20°. (Lower angles will be available after the position-sensitive detectors are checked out and installed.) Backgrounds are reasonably low, down to the lowest angle detectors, and an energy resolution of 20 meV is obtained for elastic scattering at E_0 = 500 meV, decreasing to 15 meV for an energy transfer of 300 meV. The flight-path has a cryogenic-quality vacuum (10^{-5} Torr), so that low-temperature samples can be run with a minimum of extraneous material.

Many types of dynamical investigation require large energy transfers E at relatively low momentum transfer Q. These include studies of electronic and magnetic excitations, where the form factor falls off rapidly around 2-4 $Å^{-1}$, and of molecular vibrations in fluids where recoil effects severely broaden the vibrational peaks at large Q. As an example of the latter category we show in Fig. 17 data taken on water by S. H. Chen (MIT), C-K. Loong and D. L. Price using an incident energy of 500 meV. The object of these measurements is to study the effects of supercooling on the vibrational mode around 70 meV, which may be sensitive to the more strongly correlated structure which has been observed in the supercooled state. It is seen that at Q ~ 1 $Å^{-1}$ this mode can be clearly distinguished while at larger Q it becomes completely smeared out.

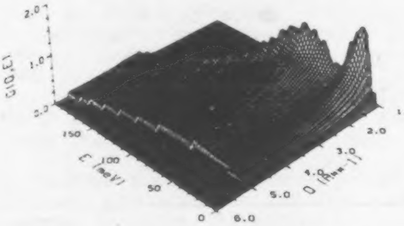


Fig. 17. The Neutron Weighted G(Q,E) from Supercooled Water (−20°C) as Measured by S. H. Chen (MIT), C-K. Loong, and D. L. Price, Using an Incident Neutron Energy of 500 meV. At small momentum transfer Q it is possible to observe a narrower peak (E ~ 30 meV) representing translational motions, and a broader peak (~70 meV) representing vibrational motions of the H_2 molecules which are the subject of this measurement. Both peaks become smeared out at larger Q.

Active scientists involved with the chopper spectrometers are C-K. Loong, D. L. Price, J. M. Carpenter, R. Kleb, and G. E. Ostrowski.

CRYSTAL ANALYZER SPECTROMETER

The crystal analyzer spectrometer (CAS), managed by T. O. Brun and R. H. Stefiuk, is presently installed at beam port F1 using the same moderator as the two powder diffractometers and LRMECS. The analyzer uses five 2 × 3 in^2 pyrolytic graphite crystals (mosaic spread 2-3°). The crystals reflect the neutrons scattered from the sample (size: 1/2 in diameter, 2 in high) onto a detector bank of seven 1/2 in diameter ^{3}He detectors. The individual detectors correspond to slightly different final energies and flight times. By combining the signal from the individual detectors, the energy resolution of the CAS is very good throughout its useful range of energy transfers (40 cm^{-1} to 4000 cm^{-1}).

During the past year, several classes of experiments have been executed: phonon density of states; hydrogen in metal; and molecular spectroscopy. From the results, it is clear that the instrument is most useful in the area of molecular spectroscopy. In particular, low lying torsional modes, which in many cases are optically inactive, have been identified. Figure 18 shows the results with no background subtraction for solid propane (only the low energy portion of the spectrum is shown). These results are part of a study of simple hydrocarbons carried out in collaboration with W. Nelligan, Schlumberger-Doll. The region 40-140 cm^{-1} is the acoustic spectrum, the two peaks at 240 cm^{-1} and 278 cm^{-1} are the two torsional frequencies, and the peak at 375 cm^{-1} corresponds to the C-C-C bend mode.

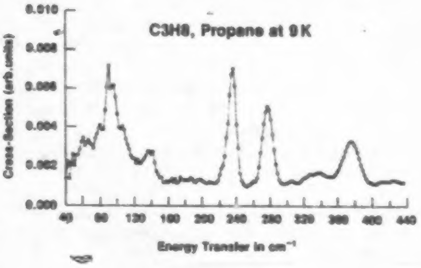


Fig. 18. Spectrum from Solid Propane.

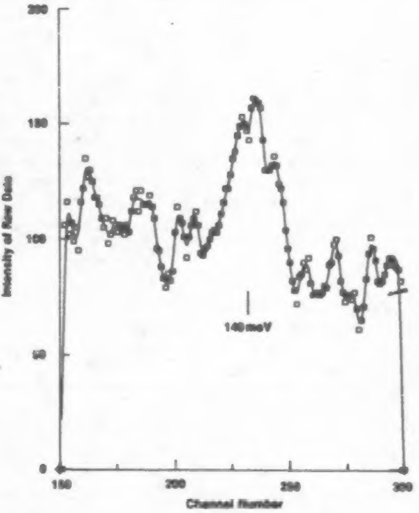


Fig. 19. Raw Data for a Ti Sample Containing 2 at% Hydrogen. Sample temperature was 20 K.

A computer program that calculates the frequencies and relative intensities for an arbitrary molecule has been installed on the IPNS VAX. Since the program was written specifically for interpreting the results for the hydrocarbons, the program uses the force field described by Schachtschneider and Snyder (SS) (Spectrochimica Acta, 19 (1963), p. 117). This SS force field is very general and can be used for molecules other than hydrocarbons. The program has been set up in format very similar to that of LAZY PULVERIX and is very easy to use.

Another example of results obtained on CAS is shown in Fig. 19, which shows raw data for a Ti sample with 2 at% hydrogen at 20 K. The peak in the data corresponds to an energy transfer of 140 meV and is the result of scattering from approximately 1 vol% of titanium dihydride precipitated in the titatium matrix. By further improvements in the background, the CAS can detect relatively small amounts of hydride precipitate in metal hydrogen systems. The results shown in Fig. 19 are part of a collaborative series of experiments with T. Rowland, University of Illinois.

eV SPECTROMETER

A prototype spectrometer for studying inelastic scattering with incident neutron energies in the eV range has been installed on beam F3. Preliminary shielding and collimation tests are now underway. This instrument will not be available for the regular user program until feasibility and adequate performance have been demonstrated. Responsible for the construction of this instrument are R. K. Crawford and J. M. Carpenter from ANL, and R. Sinclair from Harwell.

This "eV Spectrometer" uses a reverse geometry configuration with an incident white beam and monochromatic detection of the scattered neutrons. Initially the 4.28 eV resonance absorption in Ta is being used to absorb scattered neutrons in a narrow range of energies. These absorptions are detected by using scintillation techniques to detect the resulting capture gamma rays. At a later stage, other resonance absorption foils may be used (e.g., ^{238}U – 6.67 eV). Incident neutron energies are determined by time-of-flight.

The prototype instrument utilizes an incident flight path of 10 m and a 1 m scattered flight path. The prototype detector covers scattering angles from 1.4 to 2.8 degrees, making possible energy transfers up to 1 eV or more with small momentum transfers ($Q < 5$ Å^{-1}). This detector can also be placed in a backscattering configuration for large-momentum transfer studies. Energy resolution is expected to be modest (0.1-0.15 eV) in this prototype instrument.

POLARIZED NEUTRONS

Proton Polarization

Early in the lifetime of the pulsed neutron source (end of 1981) apparatus was designed and set at beam hole C2 to test a new type of neutron polarizer. This consisted of a polarized proton target, which selectively filters one spin state of neutrons of all wavelengths in the thermal and epithermal spectrum. The protons in the target were polarized by a new experimental method, called spin refrigeration. The target itself was made of a single crystal of hydrated yttrium ethyl sulfate (YES) doped with paramagnetic ytterbium. High proton polarization is achieved by rotating the extremely anisotropic crystal in a magnetic field at low temperature: the magnetic field polarizes the ytterbium impurity and, during the rotation, the polarization is transferred to the proton spins.

The tests of the proton polarization were done by transmission of a beam of cold neutrons through 1 cm thick crystal. We attained a proton polarization of 42% at 1.2 K, in a magnetic field of 14.6 kOe, rotating at 150 Hz. Such a respectable proton polarization (2/3 of the estimated electronic polarization of ytterbium) is not yet sufficient to make this device a competitive neutron spin filter, for which a minimum proton polarization of 65% is required. Extrapolation of our results indicates that this goal can be reached by increasing the magnetic field and the rotational speed by a factor of two compared with those available in our prototype device.

G. Felcher, R. Kleb, and D. Hinks have been involved in this work.

Magnetism and Superconductivity at Surfaces

Close to the surface of a magnetically active metal, the magnetic induction $\vec{B}$ is different from the bulk: we set out to demonstrate that this quantity can be measured by polarized neutron reflection. The optical principles of the experiment are quite simple: the reflectivity of neutrons is wavelength dependent and $R(\lambda)$ can be converted by an optical transformation into the refractive index $n(z)$, where z is the distance from the surface z. If the material is magnetically active, the index of refraction is spin dependent, $n(z) = n_1(z) \pm CB(z)$. Thus the magnetic induction $B(z)$ can be obtained by measuring the reflectivity of neutrons, polarized parallel and antiparallel to the net magnetization. Practically, it is possible to measure magnetic perturbation for surface thicknesses between 10 and 10^4 Å.

In the simple optical device we installed at beam hole C2, a filtered neutron beam ($\lambda > 3.8$ Å) is first polarized by reflection in a magnetized cobalt mirror; then partially reflected by the sample surface. The intensity of the doubly reflected beam is measured by a detector and the neutron wavelength determined by time of flight. The insertion of a flipping device between mirror and sample allows the reversal of the neutron spin with respect to the magnetization of the sample.

Taxing conditions are imposed on the geometrical alignment and the quality of the sample surface. A typical angle of incidence is $0.350 \pm 0.015°$. The sample surface (which should be kept in a proper magnetic field at a proper temperature) cannot conveniently exceed 2×5 cm: the size of the neutron beam does not exceed 6 mm^2. The sample surface should be microscopically and macroscopically flat and yet unstrained. It was found that this stringent requirement can be met by depositing films (>3 μ thick) on polished silicon substrates.

The first tests were done on polished surfaces of ferromagnetic NiZn ferrites: their response was almost ideal, with a magnetization at the surface quite close to that of the bulk. A more ambitious experiment was started on a film of superconducting niobium. This was cooled to 6 K and set in a magnetic field of 700 Oe, or below the critical magnetic field. The aim was to measure the penetration length of the external magnetic field into the superconducting material. The preliminary results, presented in Fig. 20, are fairly consistent with a penetration length of ~500 Å.

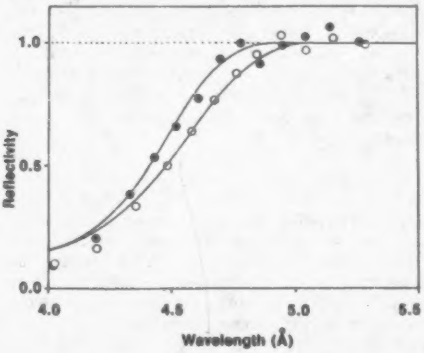


Fig. 20. Reflectivity of Nb at 6 K in 700 Oe Field, $\theta_i = 0.298 \pm 0.013°$. Data is shown for neutrons with spin parallel (open circles) and antiparallel (full circles) to the magnetic field. Curves calculated for a penetration length $\Lambda = 500$ Å.

A considerable effort is underway to improve the luminosity and efficiency of the instrument, to make it a new tool for the determination of the surface magnetic properties at the disposal of the scientific community. We are planning more definitive measurements of the magnetic fields at the surface of superconductors (including re-entrant superconductors like $ErRh_4B_4$) and, with completely different sample environment, the measurement of the surface properties of elemental ferromagnets close to the Curie temperature.

The scientists active on this surface work are G. Felcher, K. Grey, R. Kampwirth, and R. Felici.

ULTRA-LOW-TEMPERATURE DIFFRACTOMETER

An ultra-low-temperature single crystal diffractometer capable of obtaining Laue patterns from single crystals at temperatures below 1 mK has been assembled at beam hole C3. It involves the use of a dilution refrigerator, with an added nuclear demagnetization stage to cool the sample to <1 mK, and an array of 24 linear position-sensitive detectors (at a flight path of 27 cm) functioning as an effective large solid-angle area detector. To eliminate fast neutrons in the direct beam, liquid-nitrogen cooled MgO and Be filters are installed in the beam inside a shielded housing. The Fermi chopper from the old TNTOFS facility at CP-5, and a new slit package, also formed part of the original arrangement. The instrument was ready for testing in Summer 1982. The initial experiment attempted was the study of nuclear antiferromagnetic ordering in solid ^{3}He below 1 mK. This study is still making promising progress: a new sample cell is currently being designed.

Work on the diffractometer has been carried out by S. K. Sinha, *P. R. Roach, K. Sköld, B. K. Sarma, Z. Sungaila, M. Vris, J. B. Ketterson, and W. P. Halperin.

^{3}He Experiment

Studies of solid ^{3}He single crystals are an ambitious test for the ultra-low-temperature diffractometer, being an investigation of nuclear antiferromagnetic ordering below 1 mK. To get the experiment underway, elaborate preparation was required. The high-pressure container was made from single-crystal silicon to minimize background scattering — and its window successfully constructed leak-free. A vibration-free support structure was built for holding the cryostat. The refrigerator unit, which cools down to 0.05 mK, was assisted in the cooling task by two extra installations: (i) problems with heat generation from superconducting materials in the sample cell have been eliminated by inserting a magnet around the sample region to keep all materials in their normal state; (ii) heating from the neutron beam has been brought under control by filtering out the large component of γ-rays. A further requirement was a low-resolution chopper, used to search for the antiferromagnetic reflections by sweeping a monochromatic beam on the sample through a range of wavelengths. The chopper has been phased successfully with the source (the third simultaneously phased chopper to be so run at IPNS), and initial scattering experiments have been carried out from solid ^{3}He at relatively higher temperatures. The general background scattering looks encouragingly low.

The sample temperature can be measured directly by studying the transmission of neutrons of a particular spin polarization through the sample when it is slightly polarized by an applied magnetic field.

We have been fairly successful in growing these solid single crystals of ^{3}He in our specially designed sample cell (see Fig. 21). From the intensity of the (110) Bragg peak observed, we estimate this crystal fills ~1/3 of our cell. This results in a signal-to-background of ~10, which should be good enough to see the much smaller peaks expected from the spin-ordered phase.

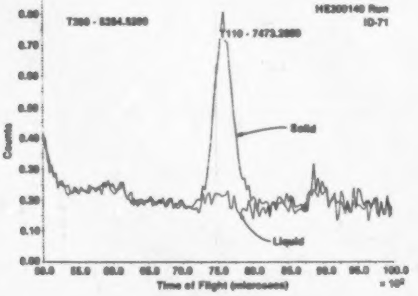


Fig. 21. Spectrum of Liquid and Single Crystal ^{3}He as Recorded in a Single Detector at the Ultra-Low-Temperature Facility. The large peak is the (110) Bragg reflection from a crystal of ^{3}He at 0.010 K.

The main question still remaining is how well the refrigerator actually cools the solid ^{3}He sample. We made an initial attempt at determining the actual sample temperature by using a $SmCo_5$ spin filter to determine the polarization of the neutron beam caused by the temperature-dependent polarization of the ^{3}He sample in a magnetic field. The results between 0.001 and 0.010 K suggest that the sample is not as cold as the refrigerator. We cannot say whether this is a result of the neutron heating or is from some other cause.

We are currently designing a new sample cell that will allow the determination of the sample temperature independent of the neutron beam. This cell will also allow us to dispense with the sample magnet which severely restricts our detector solid angle and frequently seems to block the Bragg peaks from our most easily grown large crystal.

ULTRACOLD NEUTRON EXPERIMENTS

The scientists involved with this experiment are G. R. Ringo, V. Krohn, and M. Freedman.

The ultimate aim of this experiment is to measure the electric dipole moment (EDM) of the neutron as a test of time reversal invariance. A finite EDM would show failure of time reversal. We first demonstrated a practical system for producing ultracold neutrons (UCN) at high density from a pulsed neutron source using ZING-P'. We then needed to show that we could hold these neutrons in a bottle for 100 s or so.

To do this, we (1) built a window that separates the bad vacuum of our source (a rapidly moving mica crystal which reflects 400 ms^{-1} neutrons); (2) polished the surface of our bottle; and (3) built pneumatically operated valves with minimum leakage to control the neutrons. We need a high flux of 400 m s^{-1} neutrons to test the source and bottle. For this purpose, we need and are working towards a low-temperature source: to be competitive with other measurements of the EDM, we needed a density of about 10 UCN cm^{-3} stored in our bottle.

RADIATION EFFECTS FACILITY

The Radiation Effects Facility (REF) at IPNS has been in operation since January 1982. Two fast-neutron irradiation positions operate independently at controlled temperatures between 4.2 K and about 800 K (±0.1 K). Neutron fluxes, energy spectra, and flux gradients have been accurately determined in these two temperature-controlled irradiation positions and in three ambient-temperature irradiation positions. Secondary proton and gamma fluxes have also been measured and found to be within acceptable limits. The REF is available for users' experiments approximately 1/4 of the total IPNS running time, or about 7 weeks per year.

The two primary irradiation thimbles in the REF provide fast neutron fluxes of 10^{12} n cm^{-2} s^{-1} ($E_n >$ 0.1 MeV). The access provided allows in situ measurements for the two temperature-controlled irradiation positions by two computer-controlled data acquisition systems or other electronics. A third thimble in the REF, the "rabbit," provides ambient-temperature irradiations of sample capsules without in situ measurements but sample changes can be made quickly. The neutrons in the REF have an energy spectrum quite similar to a slightly degraded fission-neutron spectrum but with a high-energy component and without a significant thermal neutron component (<2% of the fast neutron flux). Two additional irradiation thimbles in the reflector region of the Neutron Scattering Target (NST) provide ambient-temperature irradiations. The neutron energy spectrum in these thimbles is similar to the REF but with a large thermal neutron component (~77% of the fast neutron flux). A large-diameter (5 cm) thimble is being developed for ambient-temperature thermal neutron irradiations in the NSF. A 70 kG superconducting magnet is available for in situ testing during irradiations at 4 K.

Recent user experiments include:

1. Low-Temperature Deep Level Transient Spectroscopy (DLTS) on fast-neutron irradiated Si and Ge.
2. Radiation enhanced diffusion in Cu_3Au during fast neutron irradiation at temperatures between 5 and 430 K.
3. Irradiation of Epoxy and Polyimide-based insulators at 5 and 300 K.
4. Interactions of gliding dislocations with dislocation loops in neutron-irradiated niobium, vanadium alloys, stainless steel, and ferritic steels.
5. Magnetoresistivity of Cu at 5 K under cyclic irradiation and annealing.
6. Energy release during low temperature recovery in Cu.
7. Radiation hardening in fcc metals.

Defects in Silicon

Among the experimental techniques being used to study the defects introduced into Si are changes in the helium-temperature electrical resistivity. Figure 22 shows the recovery of the resistivity for n- and p-type Si after fast-neutron irradiation at liquid-helium temperature. The resistivity changes indicate the total concentration of all electrically active defects. The increases or decreases of the resistivity can be due to either changes of a defect charge state or changes in the defect concentration. DLTS is now being used to study the nature of the changes and the defects responsible for them. The recovery between 80 and 120 K appears to be associated with the annealing of the single vacancy while the recovery between 150 and 350 K involves in part the disappearance of the vacancy-oxygen complex. These experiments represent collaboration by R. Birtcher (ANL) and J. Meese (Univ. of Missouri), who spent six months at Argonne.

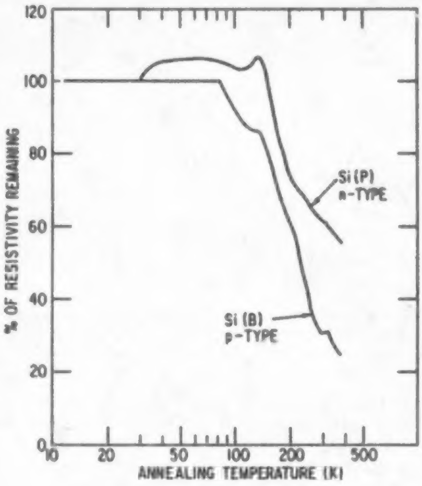


Fig. 22. Recovery of Resistivity for n- and p-type Si after Fast-Neutron Irradiation at Liquid-Helium Temperature.

Diffusion in Cu_3Au

This experiment is designed to study enhanced vacancy diffusion under fast-neutron bombardment in atomically ordered Cu_3Au. Using resistivity as a direct measure of order change during irradiation, the effects of variations in irradiation temperature, neutron dose rates, and the Bragg-Williams long-range order parameter (S) are displayed in Fig. 23. Disordering occurs within the defect cascades produced by fast neutrons and ordering occurs by free vacancy migration between cascades. (The vacancy recovery stage is centered at 300 K and the critical ordering temperature is 653 K.) Comparisons of data with the theories of radiation enhanced diffusion and ordering are in progress. Additional experiments to substantiate and expand these data are also in progress. This work has been carried out by M. Kirk.

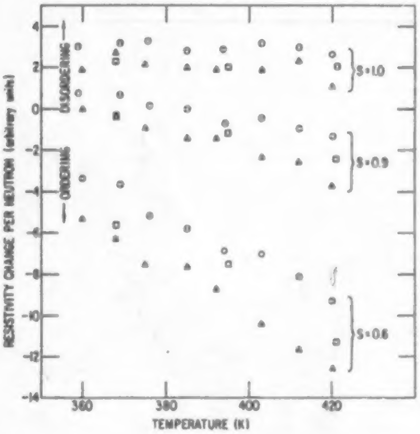


Fig. 23. Resistivity Change per Incident Fast Neutron as a Function of Irradiation Temperature in Samples of Cu_3Au with Long-Range Order Parameters (S) Shown and at Three Dose Rates as Defined by the Accelerator Frequencies: 30 Hz, ○; 10 Hz, □; and 5 Hz, △.

Critical Current Densities in NbTi

A broad spectrum of NbTi superconductors (33 single core and 3 commercial multifilamentary conductors) of various metallurgical conditions, initial Ti concentration (42, 49, and 54% Ti), annealing temperature and cold work were irradiated at low temperature (5 K) by P. Hahn and H. Weber of the Technical Univeristy of Vienna, Austria, and B. Brown. In order to reproduce the intended operating conditions of a fusion magnet, the critical current density (j_c) was measured after a series of irradiations at 4 K followed by a 24 h anneal at 300 K, for a variety of magnetic field strengths (see Fig. 24).

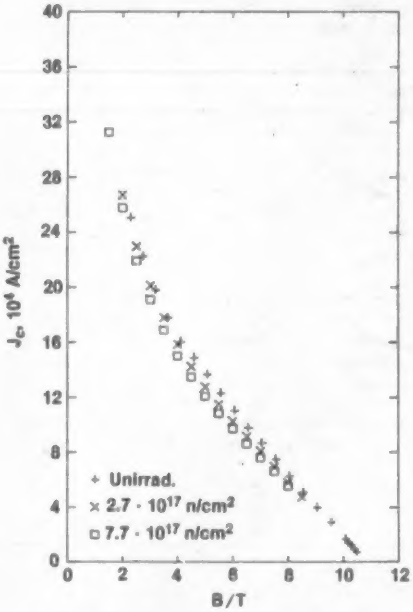


Fig. 24. Dependence of the Critical Current Density Upon Magnetic Field for Nb-49 wt% Ti Measured Following 5 K Fast Neutron Irradiation and a 300 K Anneal.

The results of 5 K irradiation available so far may be summarized as follows:

- Increases of j_c following neutron irradiation occur only in conductors which are far from the optimal metallurgical treatments.
- The changes of j_c following neutron irradiation and a thermal cycle to room temperature are small and in most cases comparable to the results obtained after 77 K irradiation.
- The data available so far indicate that the degradation of j_c at 8 T is larger by about 5-10% than the corresponding changes at 5 T at a neutron fluence of 1.3×10^{22} m^{-2} ($E > 0.1$ MeV).
- The increase of Cu resistivity is significant even after a thermal cycle to room temperature and requires design changes for a stable magnet operation.

Further experiments up to higher fluences and a detailed comparison of j_c changes following neutron irradiation with different energy spectra are under way.

RESEARCH PERSONNEL

The following represents the personnel involved in the scientific interactions at IPNS. Many are based outside the IPNS program and not all are full time working on neutrons. For current visitors at IPNS see Section 5. In those cases where scientists have instrument responsibility at IPNS, the instrument is given in parentheses.

IPNS Program

C. Loong - inelastic scattering (LRMECS)
M. Mueller - powder diffraction
F. Rotella - Rietveld analysis software

Materials Science & Technology Division

M. Arai - diffraction from glasses
M. Beno - single crystal diffraction
R. Birtcher - radiation effects (REF)
T. Brun - inelastic scattering (CAS)
J. Epperson - small angle scattering (SAD)
J. Faber - powder diffraction (GPPD)
G. Felcher - polarized beams
R. Hilleke - ultra-low-temperature project
J. D. Jorgensen - powder diffraction (SEPD)
J-E. Jorgensen - powder diffraction
M. Kirk - radiation effects
P. Leung - single crystal diffraction
D. Price - inelastic scattering (HRMECS)
P. Roach - ultra-low-temperature project
A. Schultz - single crystal diffraction (SCD)
J. Williams - single crystal diffraction

Physics Division

M. Friedman - ultracold neutrons
T. Khoe - advanced accelerator design
V. Krohn - ultracold neutrons
R. Kustom - advanced accelerator design
G. Ringo - ultracold neutrons

Electronics Division

R. Brenner - position sensitive detectors
J. Daly - interface systems
J. Haumann - interface systems
M. Strauss - position sensitive detectors

Biology Division

C. Borso - small angle scattering (SAD)

High Energy Physics

S. Kramer - proton therapy
Working occasionally on the proton test beam used for detector development are I. Ambats, D. Ayres, T. Fields, B. Musgrave, L. Price, R. Stanek, M. Marshak (Univ. of Minnesota) and R. Ruchti (Univ. of Notre Dame).

Valuable technical help is also acknowledged from the following outside IPNS.

T. Erickson - equipment maintenance
L. Funk - data handling
L. Greenwood - neutron dosimetry
R. Hitterman - data handling
M. Howe - health physics
R. Kleb - equipment design
H. Knott - data handling
B. Loomis - target design
P. Renardo - custodian
K. Sidorowicz - electronics
H. Thresh - target construction
F. Williamson - data acquisition

5. IPNS USERS

6. MEETINGS AND WORKSHOPS

7. FUTURE AND DEVELOPMENTS

5. IPNS USERS

In the table below are shown statistics of IPNS Users: the number of visits and institutions are given for the two separate years of IPNS operation. Also details of proposals are given. Along with visitors, approximately 40 scientists from various divisions within ANL are involved in IPNS experimental work, which includes the 9 Instrument and Facilities Scientists.

USERS PROGRAM

	November 1981-October 1982		November 1982-July 1983	
	Different Places	People Who Come to IPNS	Different Places	People Who Come to IPNS
US Universities	23	40	16	32
Industrial Labs	5	5	5	5
Government Labs	5	9	6	9
Foreign Institutions	8	14	15	19
TOTALS	41	68	42	65

Proposals (by principal investigator)

	March 1982	(% of Total)	November 1982	(% of Total)	June 1983	(% of Total)
ANL	36	47%	24	27%	20	26%
Outside	40	53%	66	73%	58	74%
TOTALS	76		90		78	

Collaboration and inter-laboratory exchange have always been a major part of the pulsed-neutron world effort. During the period since August 1981, we have enjoyed active programs with Los Alamos National Laboratory (LANL); the Rutherford-Appleton Laboratory (RAL); Harwell; Jülich; Karlsruhe; the Japanese KENS facility; and the ILL. These laboratories provide most of our long-term exchanges. As well as these exchange programs, the IPNS supports both collaborating (ANL plus visitor) and independent Users, whose proposals have been accepted by the Program Committee. This latter category accounts for about 20% of the experiments performed. IPNS Instrument Scientists carrying out their own experiments, together with ANL-based scientists, account for 40% of experiments completed.

A final category of User is the independent concern who buys beam time, a standard route to obtaining time when insufficient is allocated. Schlumberger-Doll (Connecticut) have bought beam time for experiments to characterize alkanes. Discussions with other organizations on purchasing proprietary time are in progress. DOE approval has been granted for these endeavors.

SPECIFIC EXCHANGES

With Los Alamos National Laboratory (LANL), we have been involved in projects on the single-crystal diffractometer, target/moderator studies, chopper and resonance spectrometers. Discussions are also in hand for making software and documentation similar at LANL and ANL. Further collaboration with LANL lies in our plans for a new eV spectrometer. Finally, from June 1983, the IPNS Program Committee began to evaluate proposals for two of the LANL instruments, thus becoming a joint Program Committee for pulsed neutron research.

Short term visitors have included B. Krause and G. Anderson (Northern Illinios Univ.) working on the SCD during the summer of 1983, G. Summerfield (Univ. of Michigan) for the summer of 1982, J. Copley (McMaster Univ.) also in 1982, and D. Mildner (Univ. of Missouri) who spends a couple of days a month at IPNS.

From England, at the **Rutherford-Appleton Laboratory** (RAL), we had visits in summer 1982 from S. Howells, who spent 3 months here, and D. Cebula for a quick experiment on the small-angle scattering diffractometer (SAD) in July 1983. A return visit by K. Crawford to RAL was paid in 1982. We are holding discussions with RAL on both position-sensitive detectors and uranium target construction.

From **Harwell**, C. Windsor visited in May 1982 and will be here again in November 1983. R. Sinclair visited in the fall of 1983, to work on the new eV spectrometer. In connection with this exchange, D. Price will be visiting England in spring 1984.

Following an experiment in April 1983, by T. Cheetham and P. Battle from the Department of Chemical Crystallography and the Department of Inorganic Chemistry, **University of Oxford**, M. Eddy also from the Chemical Crystallography Department visited for 3 months. His work involved improving software associated with the Rietveld refinement, under the guidance of F. Rotella and J. Jorgensen.

From the **Institut Laue Langevin** (ILL), we have many short-term visitors, including F. Mezei working on SAD; D. Worcester and L. Braganza also working on SAD, solving biological problems; J. Allibon, who worked here on software for six weeks; and a number of other ILL staff passed through briefly to look at the pulsed neutron business. The Argonne Electronics Division is now in the process of building a high-resolution position-sensitive neutron detector for use in Grenoble at the ILL. The contract for ANL to build this system was signed with a flurry of trumpets when the two Directors met in Grenoble in March 1983.

Moving to other European collaborations, we have had an agreement between the **Kernforschungsanlage Institut, Jülich** and the accelerator division at ANL, which provides help for the German spallation project in the form of assistance in design of a rapid cycling synchrotron for the KFA spallation neutron source [fully described in ANL Report-83-13 (1983)]. From Jülich, we had a one-year visit from M. Loewenhaupt, who was involved in a number of neutron experiments on magnetic systems.

Still in Europe, from the **University of Rome, Italy**, R. Felici is visiting for 8 months in 1983, and C. Andreani came for the month of July 1983. From the **Technical University of Vienna, Austria**, P. Hahn has completed one year of study here, working on radiation effects and H. Weber of the **Atomic Institute of the Austrian Universities**, in **Vienna**, joined the ANL team for two months.

Further afield, the **KENS** facility in **Japan** has strong connections with the IPNS. J. Carpenter from ANL spent 3 months at the Japanese KENS facility where he was involved in a number of projects including testing of a prototype resonance spectrometer. This work is joint with N. Watanabe, S. Ikeda, Y. Masuda, and S. Sato.

Furthermore, ANL has negotiated a neutron-related program between the KENS Laboratory and the Materials Science and Technology Division, for ANL to build a uranium target for the KENS facility. We have been happy to host S. Egusa from the **Japanese Atomic Energy Research Institute** (**JAERI**), who spent a year working on radiation effects, H. Horiuchi from **Osaka University** has just completed a year here working on the Single Crystal Diffractometer (SAD), and M. Arai from **Tohoku University**, who is here as a postdoctorate appointee. Also from Tohoku University, N. Niimura, K. Yamada and H. Kaneko will be visiting in late 1983 for a period of 2 months for experiments and data analysis on the single crystal diffractometer.

IPNS VISITORS

Below, we detail people who have visited IPNS to carry out experiments together with their affiliations: Involved are 32 USA Universities, 19 USA Industrial and National Laboratories; and 16 foreign Universities and 10 foreign Industrial and National Laboratories.

IPNS VISITORS

November 1981 thru October 1982

Name of Institution	User	No. of Experiments
Universities		
University of North Carolina	M. Brookhart	1*
University of North Carolina	W. Lamanna	1
University of North Carolina	M. Humphrey	1
University of Missouri	D. F. R. Mildner	1*
University of Missouri	J. Meese	4*
University of Missouri	A. Krawitz	1*
University of Missouri	F. K. Ross	1*
University of Missouri	S. Werner	1*
Ohio State University	R. Tettenhorst	2*
Ohio State University	C. Corbato	2*
University of Louisville	G. A. Lager	4*
UCLA	C. N. J. Wagner	1*
UCLA	L. Keller	1
Penn State University	J. Lannin	1*
Penn State University	L. Pilione	1
Penn State University	R. Magana	1
Penn State University	R. Newnham	1*
Penn State University	Z. Chen	1
University of Chicago	J. Kouvel	1*
University of Chicago	S. Nagel	1*
University of Chicago	L. Busse	1*
University of Texas	J. Gurak	1*
University of Texas	R. Lagow	1
University of Texas	J. Chinn	1
University of California, Santa Barbara	J. H. Kennedy	1
Augustana College	B. McCart	1*
University of Illinois	R. O. Hilleke	2*
University of Illinois	R. Simmons	2
University of Illinois	P. Chaddah	2*
University of Illinois	P. Chow	1*
University of Illinois	H. Zabel	1*
Vanderbilt University	C. Lukehart	1
Vanderbilt University	K. Srinivasan	1
Georgia Tech	P. Sutch	1*
Georgia Tech	R. Young	1*
University of Pittsburgh	G. Jeffrey	1*
Northern Illinois University	B. Krause	1*
Bronx Community College, New York	J. Fahey	1*
University of Minnesota	M. Marshak	1
University of Pennsylvania	B. Robinson	1

IPNS VISITORS

November 1981 thru October 1982

Name of Institution
Universities
MIT
MIT
MIT
Northwestern University
Northwestern University
Northwestern University
Northwestern University
Northwestern University
Colorado State University
Iowa State University
Iowa State University
Texas A & M
Florida A & M
University of California, Davis
Polytechnic Institute, New York
Florida State University
Florida State University
Industrial and National Labs
Sandia Labs
Sandia Labs
Exxon
Exxon
Exxon
Exxon
Exxon
Exxon
Exxon
3M Company
Ames Laboratory
Ames Laboratory
Ames Laboratory
Ames Laboratory
Ames Laboratory
LANL
LANL
LANL
LANL
LANL

User	No. of Experiments
C. Berney	1*
H. Becker	2
S. Chen	1*
C. Tang	1*
J. Cohen	1*
J. Ibers	1*
D. Keszler	1
D. Luzzi	2*
S. Kern	3*
R. Jacobson	1*
H. Marek	1*
F. Cotton	1
W. Tucker	1*
W. Potter	1*
R. D. Parks	1
W. G. Moulton	1
R. C. Morris	1
B. Morosin	1
R. M. Biefeld	1
R. A. Beyerlein	4*
H. S. Horowitz	1
J. M. Longo	1
A. Jacobsen	1
D. Vaughan	1
K. R. Poeppelmeir	1
M. E. Leonowicz	1
G. Christoph	2*
W. A. Kamitakahara	5*
C. Saw	6*
H. R. Shanks	1
H. Marek	1
J. D. Corbett	1
G. Hurley	2*
J. Fowler	2*
P. J. Vergamini	1*
J. Eckert	1*
A. K. Soper	1*

IPNS VISITORS

November 1981 thru October 1982

Name of Institution	User	No. of Experiments
Industrial and National Labs		
E. I. duPont	G. Stucky	2*
E. I. duPont	D. Thorn	1
E. I. duPont	J. Parise	1*
Allied Chemical	G. E. Fish	1
Geophysical Laboratory, Washington	J. Xu	1*
Schlumberger-Doll Research	W. Nelligan	1*
BNL	S. Shapiro	1*
BNL	B. Grier	1*
BNL	G. Shirane	1
SOHIO	J. F. Brazdil	1
SOHIO	R. K. Grasselli	1
Foreign		
ETH	J. Schefer	2*
ETH	P. Fischer	4
ETH	F. Stucki	1
ETH	L. Schlapbach	4
University of Geneva	K. Yvon	4
University of Geneva	J. J. Didisheim	4
New South Wales Institute of Technology	T. Sabine	3*
New South Wales Institute of Technology	J. Taylor	1
Technical University of Munich	I. Sosnowska	1*
Nuclear Research Center — Negev, Israel	H. Shaked	2
University of Bern, Switzerland	T. Armbruster	1
CRNL	S. MacEwen	3*
Universitat des Saarlandes, Saarbruchen	H. Ruppersberg	1
Uppsala University, Sweden	R. Wappling	1*
RAL	S. Howells	1*
MacMaster University, Canada	J. Copley	2*
IFF/KFA	M. Loewenhaupt	2*
IFF/KFA	P. Erhardt	1
Hebrew University of Jerusalem	A. Bino	1*
ILL	A. Hewat	3*
ILL	F. Mezei	1*
JAERI	S. Egusa	1*
Technical University of Vienna	P. Hahn	1*
CNEN, Brazil	M. P. Otero	1*

*Visitor was at ANL for at least one experiment.

IPNS VISITORS

November 1982 thru July 1983

Name of Institution	User	No. of Experiments
Universities		
Colorado State University	S. Kern	1*
Florida A & M	W. Tucker	2*
Northwestern University	D. Luzzi	2
Northwestern University	A. Golestaneh	1*
Northwestern University	C. Bartels	1*
Northwestern University	J. Tanzer	1*
Northwestern University	M. Vris	1*
Northwestern University	B. Sarma	1*
Northwestern University	B. Christ	1*
Northwestern University	W. Halperin	1*
Northwestern University	J. Ketterson	1*
University of Illinois	H. Zabel	1*
University of Illinois	P. Sokol	1*
University of Illinois	T. Rowland	1*
University of Illinois	P. Schleifer	2*
University of Illinois	R. Hilleke	1*
University of Illinois	W. Baur	1*
University of Illinois	J. Dygas	1*
University of Illinois	H. Chen	1
Texas A & M	F. A. Cotton	1
Texas A & M	P. Rudolf	1*
Texas A & M	A. Clearfield	1*
MIT	S. Chen	2*
University of Chicago	J. Ruth	1*
University of Chicago	J. Smith	1*
University of Chicago	C. A. Pelizzari	1*
Arizona State University	R. von Dreele	1*
Penn State University	C. Zhili	1
Penn State University	J. Lannin	1*
UCLA	C. Wagner	1
UCLA	G. Etherington	1*
University of Missouri	A. Krawitz	1*
University of Missouri	S. Werner	1*
University of Missouri	R. Roberts	1*
University of Pittsburgh	G. Jeffrey	1*
University of Pittsburgh	J. Ruble	1*
University of Maryland	J. Lynn	1*
Northern Illinois University	B. Krause	1*
University of Guelph	A. Soper	1*
University of Willamette	D. Montague	1*

IPNS VISITORS

November 1982 thru July 1983

Name of Institution
Universities
University of California, Berkeley
University of California, Berkeley
Industrial and National Labs
BNL
ORNL
ORNL
ORNL
IBM
IBM
Exxon
Exxon
Exxon
Exxon
Exxon
SOHIO
Institute for Cancer Research, Philadelphia
Schlumberger-Doll Research
NBS
NBS
Xerox
LANL
LANL
LANL
LANL
LLNL
Union Carbide, New York
Foreign
CRNL
JAERI
KFA
Laboratorio MASPEC del C.N.R., Italy
Laboratorio MASPEC del C.N.R., Italy
Laboratorio MASPEC del C.N.R., Italy
Technical University of Vienna
Technical University of Vienna
Osaka University

User	No. of Experiments
R. Bragg	1
L. Henry	1
S. Shapiro	1*
R. Colman	1*
C. Klabunde	1*
H. A. Mook	1
E. Ozimek	1
G. Clark	1
J. Newsam	1*
R. Beyerlein	1*
A. Jacobson	1
D. Vaughan	1
S. Sinha	1*
R. Teller	1*
J. Glusker	1*
W. Nelligan	2*
M. Rowe	1*
J. J. Rush	1
F. Galeener	1*
A. Williams	1*
R. Robinson	1*
A. Lowson	1*
J. Smith	1*
R. Scanlan	1
J. M. Bennett	1
S. MacEwen	1*
S. Eguso	2*
M. Loewenhaupt	4*
S. Rinaldi	1
F. Leccabue	1
P. Bosi	1
P. Hahn	1*
H. Weber	1*
H. Horiuchi	1*

IPNS VISITORS

November 1982 thru July 1983

Name of Institution	User	No. of Experiments
Foreign		
RAL	D. Cebula	1*
University of Oxford	A. K. Cheetham	1*
University of Oxford	M. Eddy	1*
University of Oxford	P. Bottle	1*
University of Bristol	S. Biggin	1*
University of Bristol	M. Gay	1*
University of Bristol	R. H. Ottewill	1*
ETH	J. Schefer	1*
ETH	P. Zolliker	1
ETH	P. Fischer	1
ILL	A. Hewat	1
ILL	F. Mezei	1*
ILL	L. Braganza	1*
ILL	D. Worcestur	1*
Nuclear Research Institute, Poland	K. Mikke	1*
University of Rome, Italy	R. Felici	1*
Instituto di Fisica "G. Marconi"	C. Andreani	1*
New South Wales Institute of Technology	T. Sabine	1*
Studsvik, Sweden	K. Sköld	1*
Universita di Perugia, Italy	F. Sacchetti	1

National Laboratories

BNL: Brookhaven
CRNL: Chalk River
LANL: Los Alamos
LLNL: Lawrence Livermore
ORNL: Oak Ridge

Foreign Institutions

ETH: Eidgenoessische Technische Hochschule, Zurich, Switzerland
IFF/FKA: Kernforschungsanlage Institut, Jülich, West Germany
JAERI: Japanese Atomic Energy Research Institute
RAL: Rutherford-Appleton Laboratory, England

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*Visitor was at ANL for at least one experiment.

The following four pages show the standard proposal form which must be submitted in application for beam time at the IPNS.

Proposal forms are sent to a large subset of our mailing list approximately one month in advance of each deadline. [If you have a (P) after your name on the address label you are in this "P - proposal" subset.]

The deadlines occur at approximately 6 month intervals. The next deadline for proposal forms is December 15, 1983.

RESEARCH PROPOSAL FOR THE INTENSE PULSED NEUTRON SOURCE (IPNS) AT ARGONNE NATIONAL LABORATORY (ANL)

APPLICATION FOR BEAM TIME

To apply for neutron beam time at IPNS, a proposal form must be submitted. The Program Committee meets about twice a year to consider these proposals. A copy of our proposal form is included on the following pages: these forms are available on request. A Users' Handbook is also available to those requiring more detailed information on the facilities. Proposals should be sent to:

Dr. T. G. Worlton
IPNS Scientific Secretary
Building 360
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, Illinois 60439 (312) 972-8755 or 5518

Proposals will be accepted for the following instruments:

Special Environment Powder Diffractometer
General Purpose Powder Diffractometer
Single Crystal Diffractometer
Small Angle Diffractometer
Low-Resolution Medium-Energy Chopper Spectrometer
High-Resolution Medium-Energy Chopper Spectrometer
Crystal Analyzer Spectrometer
Cryogenic Radiation Effects Facilities (2)
Ambient Temperature Radiation Effects Facilities

Some important parameters relating to instrument performance are shown in the table included in the Instrument Section 4. Additional information may be obtained from the Instrument Scientists whose names are listed in the table.

Those who have already run experiments must submit the standard (less than 2 page) report. Forms are available from the Scientific Secretary. Further beam time will not be granted on a particular problem unless a report is submitted.

Assistance for University Users of IPNS

A policy has been established with the University of Chicago for IPNS User assistance. All IPNS Users from universities can stay at the ANL lodging facilities for 1/2 of the normal cost. A limited amount of money is available to provide full housing, travel and a $15/day living allowance for all university Users who do not have sufficient university or grant funds for travel and living expenses. Standard travel procedures (no first class travel, expense receipts, etc.) will be applied.

We would like to acknowledge the generosity of the University of Chicago here: through them we have acquired a car for IPNS Users.

PURCHASE OF PROPRIETARY BEAM TIME

Beam time for experiments on the neutron scattering instruments can be purchased under a rate structure approved by the Department of Energy (DOE). For proprietary work or publishable work that is not of direct interest to the DOE, the full cost recovery rate of $2400/instrument/day (24 hours) will be applicable. The Federal rate of $1570/instrument/day will be used for research which is of direct interest to the DOE. Experimenters desiring to carry out non-publishable research requiring beam time in excess of that assigned by the Program Committee should contact the IPNS Operations Manager, Bruce Brown, at (312) 972-4999.

EXPERIMENTAL DETAILS

☐ Scattering Experiment

1. Instrument (configuration required) ____________________
2. Estimated beam time (days) and sample size ____________________
3. Special facilities and/or equipment required from ANL ____________________
4. Range of momentum and energy transfer required ____________________
5. Momentum and energy transfer resolution required ____________________
6. Space group ____________________
7. Cell dimensions ____________________
8. Safety concerns (any potential hazards) ____________________

☐ Radiation Effects Experiment

1. Is temperature control required? If so, in what range? ____________________
2. Are in-situ measurements involved? ____________________
3. Facility/Number of separate irradiations ____________________
4. Requested time (days) ____________________
5. Special facilities and/or equipment required from ANL ____________________
6. Safety concerns (any potential hazards) ____________________

☐ Special Experiment

1. Beam or moderator required ____________________
2. Estimated length of experiment (months) ____________________
3. Special facilities and/or equipment required from ANL ____________________
4. Safety concerns (any potential hazards) ____________________

REASONS FOR USING A PULSED NEUTRON SOURCE

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PROPOSED EXPERIMENT (no additional sheets may be used)

Writing Good Proposals for the IPNS Facility

We have found that some proposals submitted for consideration by the IPNS/LANL Program Committee are poorly written, thus diminishing the chance for their acceptance. This note is intended to assist prospective IPNS Users in writing better proposals.

It is particularly important to include an explanation of your reasons for wanting to use a pulsed neutron source as opposed to using x-rays, a reactor neutron source or some other experimental technique such as NMR, Infrared, or Raman measurements. If you are not sure of the need to use a pulsed neutron source it might be helpful to discuss your proposal with the appropriate Instrument Scientist before submitting it.

Under the Proposed Experiment section you should give a short explanation of the scientific basis for the experiment, along with a brief history and/or discussion of related measurements. If the proposal is a continuation of a previous IPNS measurement, please indicate this on the front of the form and add the proposal number of the previous measurement. In this case we must have a report of the first measurement before the continuation proposal can be considered.

Under the Experimental Details section be sure to specify the proposed instrument and the desired beam time. You may use a generic name (i.e. "Powder Diffractometer" or "Chopper Spectrometer") to specify a given instrument type when more than one of that type of instrument exist at the facility at which you hope to perform the measurements and you are undecided as to which of the instruments to use. When you specify a generic instrument name in your proposal, the actual instrument to be used will be decided by the Program Committee or the Scheduling Committee and you will be notified of this decision when your experiment is scheduled. The desired beam time should always be specified in days unless the proposed measurement is to use an uninstrumented neutron beam, in which case beam time should be specified in months. If you are unsure of beam time required, again consult our Instrument Scientists. It is also important to note any special ancillary equipment that may be needed for the measurement and the desired operating conditions of this equipment.

In the case of a proposal covering measurements on multiple samples or multiple measurements on the same sample under different experimental conditions, make sure that the number of measurements to be performed and the desired beam time per measurement are clearly indicated in the proposal, along with the total beam time needed to complete the entire proposal. If you are proposing to use more than one instrument for a series of measurements, please submit separate proposals for each instrument and make a note about the companion measurements on each proposal. It is usually a good idea to end the proposal with a few pertinent references. References to unpublished work are acceptable only in the sense that you indicate that you have a scientific program on this subject. To reference unpublished work as a key element of your proposal acts only to frustrate a Program Committee. It is better to spell out the results clearly.

Remember that your proposal will be in competition with other proposals and not all can be accepted even when they are all excellent, so do not diminish your chances of acceptance by submitting a proposal which does not contain all the needed information.

Please return completed form to: IPNS Scientific Secretary, Bldg. 360, Argonne National Laboratory, Argonne, IL 60439.

ACTIONS TAKEN

Proposal No. ______________________

Proposed Instrument ______________________

1. Review by Operations

☐ Facilities requested are available, with exceptions as noted below.

☐ Facilities requested not available.

Comments ______________________

____

____

2. Review by Program Committee on ______________________.

☐ Accepted for ________ days, on the ______________ instrument with conditions as noted below.

☐ Accepted as back-up experiment on the ______________ instrument.

☐ Not accepted for this period.

Comments ______________________

____

____

3. Program Committee decision communicated to user

Date ______________ By ______________

4. Scheduling Committee action

Scheduled for ______________ days starting ______________

5. Scheduling decision communicated to user

Date ______________ By ______________

6. Operating time

Run for ______________ days starting ______________

7. Report on experiment

Date ______________ By ______________

in form of ______________________

PROGRAM COMMITTEE FOR IPNS AND LOS ALAMOS WNR PULSED NEUTRON FACILITY

J. M. Rowe (Chairman)	Reactor Radiation Division, NBS
J. D. Axe	Physics Dept., Brookhaven National Laboratory
W. L. Brown	Radiation Physics Dept., Bell Laboratories
J. B. Cohen	Dept. of Materials Sciences & Engineering, Northwestern University
J. Eckert	Physics Division, Los Alamos National Laboratory
P. A. Egelstaff	Dept. of Physics, Univ. of Guelph, Canada
D. M. Engelman	Dept. of Molecular Biophysics & Biochemistry, Yale University
R. L. Harlow	E. I. du Pont
G. A. Jeffrey	Dept. of Crystallography, Univ. of Pittsburgh
J. D. Jorgensen	Materials Science & Tech. Division, Argonne National Laboratory
M. Kirk	Materials Science & Tech. Division, Argonne National Laboratory
B. Larson	Solid State Division, Oak Ridge National Laboratory
L. Passell	Physics Dept., Brookhaven National Laboratory
D. L. Price	Materials Science & Tech. Division, Argonne National Laboratory
P. J. Vergamini	Physics Division, Los Alamos National Laboratory
	Past Members
T. H. Blewitt	Materials Science & Tech. Division, Argonne National Laboratory
L. Eyring	Dept. of Chemistry, Arizona State Univ.
S. Krimm	Dept. of Physics, Univ. of Michigan
J. P. McTague	Dept. of Chem., UCLA, now at Brookhaven National Laboratory
S. K. Sinha	Materials Science & Tech. Division, Argonne National Laboratory, now at Exxon R&D Laboratory
C. Stassis	Dept. of Physics, Iowa State Univ.
S. A. Werner	Dept. of Physics, Univ. of Missouri
J. M. Williams	Chemistry Division, Argonne National Laboratory
F. W. Young	Solid State Division, Oak Ridge National Laboratory

6. CONFERENCES AND WORKSHOPS

The Conferences and Workshops held have been in both general and specialist areas. Workshops have been held jointly with Los Alamos National Laboratory, and one is planned at NBS, Washington. Financial and technical assistance from both the University of Chicago and the Division of Educational Programs (ANL) for these conferences and workshops is gratefully acknowledged.

CONFERENCES AND WORKSHOPS

July 20-24, 1981	Faculty Institute: The Intense Pulsed Neutron Source
August 12-14, 1981	Int. Symp. Neutron Scattering
November 9-12, 1981	Int. Conf. Neutron Irradiation Effects in Solids
May 20-21, 1982	Workshop: Resonance Neutron Radiography
June 9-11, 1982	Faculty Institute: Introduction to X-ray and Neutron Diffraction in Biology, Chemistry, and Materials Science
June 27-July 2, 1982	ICANS-VI (International Collaboration on Advanced Neutron Sources)
July 13-16, 1982	Workshop: Powder Diffraction and Rietveld Analysis
June 27-29, 1983	Workshop: Application of Neutron Scattering to Chemistry (joint ANL, LANL)

PLANNED MEETINGS

November 15-16, 1983	User Meeting
November 17-18, 1983	Workshop: Applications of Neutron Scattering to Engineering Materials
February 13-15, 1984	Workshop at LANL: High Energy Excitations (joint ANL, LANL)
April 2-4, 1984	Workshop at NBS: Powder Diffraction (to be held in collaboration with ANL)

Below are descriptions of the meetings listed in chronological order.

Faculty Institute

About sixty scientists from universities and other research laboratories were at Argonne July 20-24 to attend a Faculty Institute on the Intense Pulsed Neutron Source, sponsored by Argonne's Division of Educational Programs through its Materials Sciences Committee and by Argonne Universities Association. Dr. Robert W. Springer, Director of the Division of Educational Programs, and Dr. Henry V. Bohm, the President of the Argonne Universities Association gave welcoming remarks to the attendees. The Institute started with introductory talks about Argonne facilities and tours of selected Facilities. Highlights of the Institute included an "Introduction to Neutron Scattering" by Professor Clifford Shull of MIT (one of the early pioneers in neutron scattering) and an "Introduction to Radiation Effects" by Professor Werner Schilling of Julich, West Germany. Professor Christian N. J. Wagner of UCLA spoke on Amorphous Systems, Professor Lyle Schwartz of Northwestern University on Phase Transformations in Alloys, Professor E. Morton Bradbury of the University of California at Davis on Biological Applications of Small Angle Scattering, Dr. Robert Ward of the University of Missouri on Resonant Neutron Scattering as a Probe of Condensed Matter, and Professor Samuel A. Werner of the University of Missouri on Magnetism.

Argonne speakers at the Institute included Mr. A. B. Krisciunas and Drs. F. Y. Fradin, R. C. Pardo, J. J. Katz, D. L. Price, B. S. Brown, T. H. Blewitt, A. J. Schultz, J. M. Williams, M. H. Mueller, J. D. Jorgensen, R. C. Birtcher, J. Faber, J. E. Epperson, C. S. Borso, G. P. Felcher, and T. O. Brun.

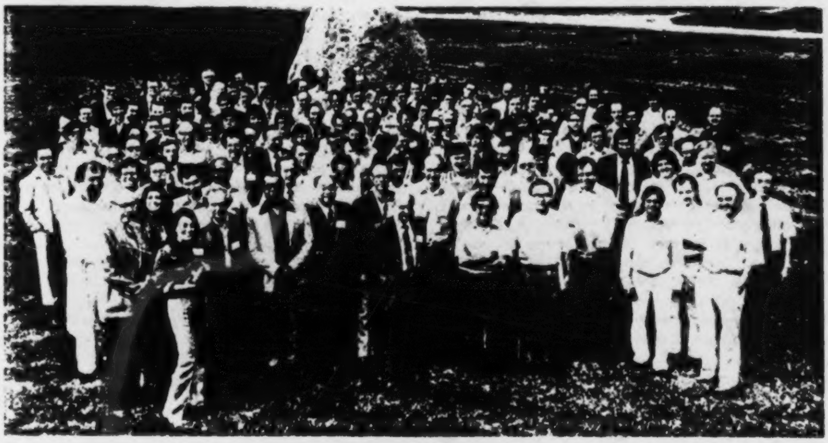
International Symposium on Neutron Scattering

This Symposium was held in conjunction with the International Crystallography Congress in Ottawa. The meeting was attended by some 148 scientists working in the field of neutron scattering, 63 of whom came from overseas. In addition to sessions of invited talks in the areas of Pulsed Neutron Research, Instrumentation and Techniques, Small Angle Scattering and Biology, Magnetism, and Disordered Solids there was a poster session of contributed papers. There was a conducted tour of IPNS for the conference attendees on the afternoon of August 13.

Am. Inst. Phys. Conf. Proc., Vol. 89, AIP, New York, 1982.

International Conference on Neutron Irradiation Effects in Solids

This meeting, co-chaired by T. Blewitt and B. Brown, was attended by more than 100 scientists working in various fields of radiation damage representing 11 countries. There is currently a growing tendency to replace research reactors with charged particle accelerator based sources such as the FMIT at Hanford, the IPNS at Argonne, and similar machines in Japan and Europe. If these machines are to be used as neutron sources for basic irradiation studies, they will represent new challenges and new opportunities for radiation effects research. The conference was ac-



Symposium on Neutron Scattering
August 12-14, 1981
Argonne National Laboratory
Argonne, Illinois U.S.A.

International Conference on
Neutron Irradiation Effects in Solids
November 9-12, 1981
Argonne National Laboratory
Argonne, Illinois U.S.A.

cordingly organized specifically for an assessment of the field in order to evaluate the neutron source needs of the research community and to determine to what extent they could be satisfied by the accelerator based sources. The program included sessions with invited and contributed talks on Cascade Studies and Ion Simulation, New Neutron Sources, Radiation Effects in Fusion and Breeder Reactors, Fusion Magnet Materials, Irradiation Induced Changes in Mechanical Properties, Fundamental Radiation Effects in Metals, Void Effects, and Semiconductors and Ceramics. There was a poster session in the main IPNS control room followed by tours of IPNS.

J. Nucl. Mater., 108 and 109 (1982).

Workshop on Resonance Neutron Radiography

Some 25 people with interest in neutron radiography from industry, national laboratories (including Europe) and universities met together to discuss the potential applications of Resonance Neutron Radiography. The local organizer was M. G. Strauss.

Resonance Neutron Radiography (RNR) is a nondestructive analytical technique in which separate images of the spatial distribution of different isotopes within an object can be obtained with a single neutron exposure. The isotopic selectivity of RNR is achieved by virtue of the greatly increased absorption of neutrons by sample nuclei at specific resonance energies. Although the feasibility of RNR has been recognized before, the means for making it a practicable NDE technique were not available until two recent developments at Argonne: (1) an intense source of pulsed epithermal neutrons (IPNS) and (2) a neutron position-sensitive scintillation detector with high efficiency in the epithermal range.

Discussions on general applications of RNR were led by Harold Berger (Industrial Quality, Inc., Gaithersburg, MD) and covered such areas of analysis as elemental distribution in chemicals and metallurgical samples, e.g., hafnium in steel, and evaluation of material deposition in plating processes such as uniformity of thin films. Applications of RNR in the nuclear fuel field appeared most promising. Discussions in this area were led by John Barton (N-Ray Engineering Co., La Jolla, CA). These applications are based on the capability of the technique to simultaneously image the isotopes of uranium and plutonium and those of fission products.

The workshop made it apparent that RNR will be cost effective only where high reliability, and therefore quality control, are imperative such as in nuclear power and space applications. Experiments in these areas would show where the unique capabilities of this technique could be brought to bear with advantage.

Interim ANL Report: Abstract of ANL Workshop on Resonance Neutron Radiography, May 20-21, 1982.

Faculty Institute

The Institute, entitled "An Introduction to X-ray and Neutron Diffraction in Biology, Chemistry, and Materials Science," was held at Argonne under the auspices of the Division of Educational Programs. Local organizers were J. M. Williams, J. Faber, and M. Schiffer. The purpose of the Institute was to provide an introduction to diffraction methods, and their application, because the results of diffraction experiments have an ever increasing impact on a variety of modern research disciplines. The Institute was attended by approximately 35 scientists representing a wide range of scientific disciplines. Invited lecturers from outside ANL included J. B. Cohen of Northwestern University and F. K. Ross of The University of Missouri. In addition to lectures and x-ray laboratory demonstrations, a visit to the IPNS was also made.

ICANS-VI

Sixty participants from eleven laboratories and several firms came to Argonne for the sixth meeting of the International Collaboration on Advanced Neutron Sources, organized by J. M. Carpenter. On the first day we heard status reports on spallation source projects at six laboratories.

SNS, Rutherford Appleton Laboratory, UK, Gray

KENS, KENS-I' and KENS-II, Laboratory for High Energy Physics, Japan, Watanabe

SNQ and SNQ', Kernforschungsanlage, Julich, Germany, Bauer

WNR and WNR/PSR, Los Alamos National Laboratory, Silver

SIN Thermal Neutron Source, Swiss Institute for Nuclear Research, Fischer

IPNS, Argonne National Laboratory, Lander

In addition Bauer reported recent Soviet neutron source developments, summarized from the June 1982 Dubna meeting. We devoted the rest of the week to technical reports, and working discussions about Targets and Moderators, and Neutron Scattering Instruments. The reports showed a continuing rapid progress in the work in the year since the last meeting at Julich and Karlsruhe and a number of collaborative efforts were identified.

ANL Report ANL-82-80 (1983).

6th Meeting of the International
Collaboration on Advanced Neutron Sources
June 28-July 2, 1982
Argonne National Laboratory
Argonne, Illinois U.S.A.

Powder Diffraction and Rietveld Analysis Workshop

IPNS and the Division of Educational Programs cosponsored this short course which was organized locally by F. J. Rotella, J. D. Jorgensen, M. H. Mueller, and J. Faber, Jr. The course was designed to appeal not only to scientists who routinely refine crystal structures from powder diffraction data via the Rietveld method, but also to researchers who have only a casual acquaintance with this area.

A series of lectures on basic topics was presented which included: Fundamentals of Neutron Diffraction, Fundamentals of Non-linear Least-Squares Minimization of Diffractometer Design and Fundamentals of the Rietveld Method as Applied to Conventional and Pulsed Neutron Sources, along with topics of interest to those students with a background in powder diffraction and its applications including Total Pattern Refinement, Solving Unknown Structures from Powder Data, Application of the Rietveld Method to Conventional and Synchrotron X-ray Sources, Scattering from Amorphous Solids and Liquids, Bulk Strain Studies with High-Resolution Neutron Powder Diffraction and Magnetic Structures. Lecturers included: T. M. Sabine, New South Wales Institute of Technology, Australia; A. W. Hewat, Institut Laue-Langevin, France; E. Prince, National Bureau of Standards, USA; R. B. von Dreele, Arizona State University, USA; R. A. Young, Georgia Tech., USA; D. E. Cox, Brookhaven National Laboratory, USA; J. R. D. Copley, McMaster University, Canada; S. A. MacEwen, Chalk River National Laboratory, Canada; and J. Faber, Jr., G. P. Felcher, and J. D. Jorgensen, Argonne National Laboratory, USA.

In addition to these lectures, the students were given "hands-on" experience in the collection and analysis of powder data at the IPNS facility. Sintered samples of $A\ell_2O_3$ were used to show the students the proper method for loading a sample and collecting data on the General Purpose and Special Environment Powder Diffractometers. The high-resolution powder data collected on these instruments were transferred to the VAX-11/780 computing system used at IPNS, and the students refined the crystal structure of $A\ell_2O_3$ from "their data" under the supervision of local staff using the Rietveld analysis package of computer programs maintained on the IPNS VAX. Within a matter of two afternoons, the students were able to learn how to use the local Rietveld computer codes and to carry a relatively simple structural analysis to completion.

In all, 48 scientists whose research interests range among chemistry, geology, materials science and physics were officially registered as students for the short course, 29 of whom were not associated with Argonne.

Feedback from students and lecturers alike indicated to the organizing committee that the short course was instructional and served as a forum for state-of-the-art powder-diffraction. Two direct results have originated from the Workshop, first, the invited lecturers are actively considering putting together the first book on the broad applications of the Rietveld method and, second, five new proposals have arrived at ANL for research at IPNS from scientists who attended the Workshop.

Workshop on the Application of Neutron Scattering to Chemistry

This workshop was hosted by IPNS with financial support from the University of Chicago and administrative assistance from Argonne's Division of Educational Programs. The workshop was a joint venture with Los Alamos National Labortory and we were pleased to welcome J. Eckert and P. Vergamini onto the Organizing Committee consisting of T. Brun, A. Schultz, P. Leung, M. Mueller, and F. Rotella from ANL. Sixty-one participants attended the workshop, almost all from University departments from as far afield as Arizona State University and the University of Virginia. Invited lecturers and topics presented included: H. Fuess from University of Frankfurt gave an introduction to neutrons and also talked on charge and spin densities; F. Ross from University of Missouri, Columbia, introduced crystallography and talked on H-bonded systems; J. Howard from University of Durham, England, introduced molecular spectroscopy and talked on studies of catalysts; C. Strouse from UCLA talked on the applications of crystallography to structure and bonding; A. Dianoux from the Institute Laue-Langevin, Grenoble talked on the principles of quasi-elastic scattering and recent studies with this technique; S. Yip from MIT discussed the analysis and interpretation of neutron inelastic scattering spectra; and J. Faber, Jr. and J. D. Jorgensen, both from Argonne, gave an introduction to neutron powder diffraction and spoke on recent structural studies from neutron powder data using time-of-flight Rietveld analysis.

The afternoon sessions were devoted to practical classes highlighting three of the time-of-flight instruments at IPNS (crystal analyzer spectrometer, general purpose powder diffractometer and single crystal diffractometer), and general discussions of both elastic and inelastic scattering from chemical systems. This required quite complex logistics since our philosophy was to give each participant the opportunity to understand, if only at preliminary level, what the instruments could do.

By general consent the workshop was a success, with lots of questions, including requests as to how to submit proposals to the IPNS and WNR pulsed neutron facilities.

7. FUTURE PLANS FOR IPNS

In the two years of operation of IPNS, we have learned a good deal: in particular we have been able to determine which relatively modest improvements will lead to the highest gain in scientific output. These improvements fall into four areas.

ENRICHED TARGET SYSTEM AND NEW NEUTRON COLD MODERATOR

The IPNS target facility has performed impeccably since installation. We are already embarked on studying what is required to install an enriched uranium target at IPNS. Safety analysis studies and neutronics calculations are in progress, and the preliminary estimates are that we can have the target installed and operating by January 1985. Calculations show that this will give a factor of from three to five in intensity with no appreciable loss of resolution due to pulse width broadening and no meaningful increase in the delayed neutron background. The completion of the enriched target assembly, which will be built by Argonne, is our highest priority. No enriched target assembly operating at the projected current level now exists in the world and, thus, this effort represents an important technological experiment as well as a "flux enhancer."

Argonne experience with cold moderators at IPNS has been salutary, even if not wholly successful. The initial liquid methane design represented a compromise too heavily weighted toward intensity with unacceptable sacrifice of pulse width, reflecting the paucity of information available at the time of the moderator design (1980). At the present time we have installed two separate cold (~90 K) moderators, one for the ultracold neutron experiment and one for the three instruments (small-angle diffractometer, polarized neutron beam and ^{3}He project) that require the long wavelength neutrons from the cold moderator and are not affected by pulse width degradation. In 1986 we plan to install a new cold (20 K) moderator assembly for these instruments and for the chopper spectrometers. Heterogeneously poisoned moderators will be used for some of the instruments. Experience is continuously being gained on moderator design at IPNS as well as at the KENS facility in Japan and the Spallation Neutron Source at Rutherford, UK.

RCS MODIFICATIONS

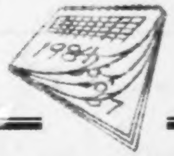
The Rapid Cycling Synchrotron (RCS), the world's highest intensity proton synchrotron, is now running reliably with 10-12 μA averages and short-term records of 13.9 μA. By mid-May of 1983, 500 million pulses had been accelerated to the target. As operating experience accumulates on this machine, however, a number of subsystems have been identified, which could be improved to enhance operating efficiency and reduce irradiation of components. Modifications should be made to the RCS to provide lower losses and activation of components and better control of the accelerated beams. These improvements will translate directly into more reliable operation and higher average beam current on target.

This program consists of three major parts: a third rf cavity will be added to help contain the beam during the early part of the cycle and prevent acceleration losses, orbit correction magnets will be added to control the beam position at low energies, and a new choke for the ring magnet power supply will provide significant improvements in stability at injection. These three items should be accompanied by continuing improvement of the RCS beam diagnostics, controls, and power supply stability.

These modifications will be handled in a fashion consistent with the fact that the RCS is scheduled to run only until the completion of the prototype FFAG accelerator.

UPGRADE OF IPNS INSTRUMENT PACKAGE

The seven user instruments, the radiation effects facility, and the three special experiments are all working well. Since many of these instruments were the first of their kind in the world, it is not surprising that, after almost two years of operation, improvements can readily be identified in a number of them. Similarly, the data acquisition system, which has functioned extremely well, requires upgrading to handle the foreseeable additional load.



Specifically we propose to:

(a) Complete the installation of the high-angle flight path of the High Resolution Medium Energy Chopper Spectrometer (HRMECS); equip the spectrometer with a full complement of detectors at small angles, and an adequate number of detectors at large angles. The larger momentum range made possible by the extra large-angle detectors is essential for studies of atomic dynamics in condensed matter at higher resolution than is possible at the Low-Resolution Medium-Energy Chopper Spectrometer (LRMECS). The additional detectors at small angle will double the counting rates in measurements of magnetic scattering, which are so far unique and at present very difficult.

(b) Upgrade the small-angle diffractometer, which has already proved valuable in biological and polymer science, by increasing the flight path, acquiring a new detector, and installing a section of guide tube.

(c) Upgrade the single-crystal diffractometer by increasing the flight path, adding another detector, improving the electronics on both detectors, and increasing the dedicated computer capability at the front end.

(d) Build one new instrument to perform quasi-elastic scattering studies from polymer, biological, and chemical systems. This instrument will be installed on a neutron guide tube from the cold moderator and thus will see a high flux of long wavelength neutrons.

(e) Increase significantly the capability of the data acquisition system including new front-end computers (some instruments currently share front-end computers, a decision forced by budget constraints in 1979 and 1980), new PDP computers for the eV spectrometer and quasi-elastic machine, and a new VAX system for data analysis. It should be realized that time-of-flight instruments with multiple-counter (especially two-dimensional) assemblies produce large quantities of data that must be processed by sophisticated computer systems. This is particularly important when we are dealing with a large throughput of outside users, and essential for rapid data analysis.

NEW ACCELERATOR SYSTEMS — CONSTRUCTION OF A PROTOTYPE FIXED-FIELD ALTERNATING GRADIENT ACCELERATOR

Looking to the future, the US will have to start planning for a new neutron source for the 1990's, and a team at ANL under the leadership of R. L. Kustom of the Physics Division has been working on advanced source concepts for some years. Having examined a number of alternatives, this team concluded, consistent with the developing international picture, that spallation sources afforded the greatest promise. Furthermore, they have proposed a new system based upon a fixed-field alternating gradient (FFAG) proton accelerator as the heart of the intense neutron source.

We will not describe in detail the FFAG design here [see R. L. Kustom (1981)], except to note some of the pros and cons. Major advantages are that the FFAG uses dc magnets, which make it possible to optimize operation of the radiofrequency cavities and to use metal vacuum chambers, the rf is used about three times as efficiently as in a rapid cycling synchrotron, and the injection process is very efficient because it is done into a dc field at 200 MeV allowing direct H^- to H^+ stripping and adiabatic capture with flexible rf programming. Finally, the FFAG is cheaper than any other machine of comparable intensity level of $>10^{17}$ n cm^{-2} s^{-1} in peak thermal flux.

However, this machine represents innovation in the area of high current accelerators. After looking critically at this reality, the design team has concluded that a small-scale prototype would provide the data necessary to produce with confidence a definitive design for the 10^{17} source. The critical components that would be tested with this prototype are related to magnet design and performance, and the methods of stacking the beam so that the effective frequency for experimentalists can be reduced to 60 Hz.

The intent of building a prototype is to provide a configuration affording critical tests of the principal ideas, and to do this in such a way that the prototype is an important scientific entity in its own right. The new prototype machine proposed for IPNS replaces the present rapid cycling synchrotron and would deliver ≅100 μA of protons at 500 MeV to the (modified) IPNS target station. A schematic of the mini-FFAG machine, and where it would be located with respect to IPNS, is shown in Fig. 25.

Finally, we summarize the IPNS improvements and modifications through their effect on the peak thermal neutron flux, starting with the current value of 4×10^{14} n cm^{-2} s^{-1}.

- the enriched target will increase this to 1.5×10^{15},
- the RCS improvements will further increase this to 3×10^{15}, and
- the prototype FFAG will bring this value to 1×10^{16}.

This progression is also shown in Fig. 26, together with the planned chronology for the entire upgrade.

R. L. Kustom, IEEE Trans. Nucl. Sci., NS-28 (1981) p. 3115.

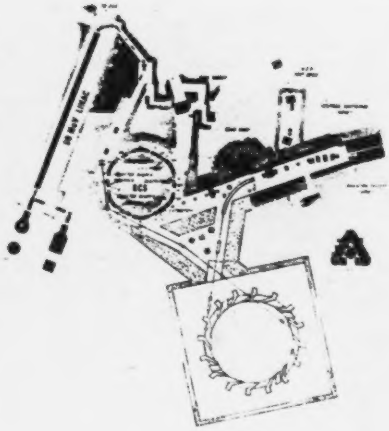


Fig. 25. Schematic of the Mini-FFAG Machine.

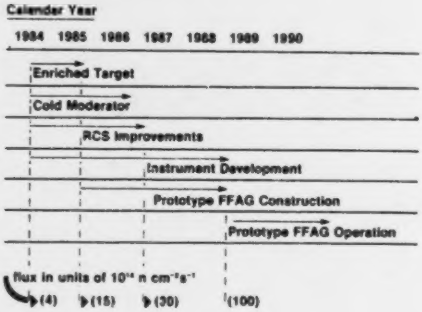
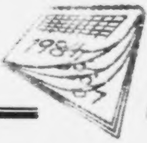


Fig. 26. IPNS Upgrade Plans.



Odds & Ends
(Anonymous)

First an important note on our existence (or not!). When Anonymous learned of the proposed Progress Report, we naturally met to discuss the expansion and amplification of the small part we are always allowed in the Bulletin. Imagine our horror when we were told, no "odds and ends" permitted in a serious report. Appealing to our many admirers around the world (incognito of course) we received a torrent (well — three actually) of letters of support. Armed with these, and our own computer generated support, we are happy to report that — as you see — we survive.

Impressed, indeed overwhelmed, by the intense activity over the Report and furious figure hunting, etc., we looked through our own extensive catalogue and decided not to be outdone. The first figure shows that our Program Director (the slightly older one) has many talents and can actually be kept in one place if a 30 lb. cast or lead shielding block (private communication) is applied. We have as yet not received the experimental report from David Stirling (the younger one in the picture) on our Director's performance.

The second figure shows the great advantages of being Facilities Manager (the one in the middle). This photo was snapped at Open House when we had (supposedly) 900 visitors. The two charming, elegant, and efficient helpers were serving as popcorn poppers but also double as IPNS Secretaries.

A third figure of our Technical Director running along beside his previous car to start it and then jumping in, seems to have unaccountably disappeared from our files. It showed, we think, the essence of technical direction. A slightly newer car can now be seen, bringing the total investment of our three leaders up to ~$1,000. Since the move (see August 1983 Bulletin) to Building 360 provided us with enormous offices and clearly new "status," Anonymous has been expecting Jaguars and BMW's but the old junk remains. In fact, the only respectable car is that from the University of Chicago for our users. We bow in amazement at the administrative genius of our Operations Manager for this coup.

Free
Heritage

We are now fully installed in Building 360 and "at home" to visitors anytime; of course, it's the office with no name on the door.

8. PUBLICATIONS

8. PUBLICATIONS

THE IPNS

General

Pulsed Spallation Neutron Sources for Condensed Matter Research, D. L. Price, Bulletin Am. Phys. Soc., 25 (1980), p. 794 [ABSTRACT].

Status of Argonne's Intense Pulsed Neutron Sources, J. M. Carpenter, Proc. 5th Int. Collaboration on Advanced Neutron Sources, June 1981, pp. 33-52.

The Argonne Pulsed Neutron Source Program, J. M. Carpenter, R. K. Crawford, S. W. Peterson, M. H. Mueller, J. D. Jorgensen, and A. H. Reis, Jr., Proc. Symp. Neutron Diffraction, Int. Union Cryst., Cracow, August 1978, Jagellonain University Press, 1981, Vol. 18, pp. 33-44.

The Area Radiation Monitor at the IPNS, J. J. Eichholz, F. J. Lynch, R. L. Mundis, M. L. Howe, and E. H. Dolecek, Proc. IEEE Nucl. Sci. Symp., October 1981, San Francisco, CA.

Pulsed Neutron Sources for Condensed Matter Research, D. L. Price, IEEE Trans. Nucl. Sci., NS-28 (1981), pp. 1661-1664.

Inelastic Scattering Measurements with 0.1-1 eV Neutrons at IPNS-I, D. L. Price, T. O. Brun, J. M. Carpenter, R. K. Crawford, C. A. Pelizzari, and S. K. Sinha, Program and Abstracts. Conf. Neutron and Its Applications, Cambridge, England, September 1982, p. 57 [ABSTRACT].

Pulsed Neutron Techniques for Condensed Matter Research, B. S. Brown, J. M. Carpenter, J. D. Jorgensen, D. L. Price, and W. Kamitakahara, in **Novel Materials and Techniques in Condensed Matter**, G. Crabtree and P. Vashishta (Eds.), 1982, pp. 311-340.

Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory (ANL): A Status Report as of June, 1982, J. M. Carpenter, C. W. Potts, and G. H. Lander, ICANS-VI Meeting, ANL, June 27-July 2, 1982, ANL Report ANL-82-80 (1983), pp. 77-101.

Pulsed Neutrons: One Year of Experience with the New Source at Argonne National Laboratory, G. H. Lander, Physica, 120B (1983), pp. 15-24.

Status Report and Future Plans of the Intense Pulsed Neutron Source — ANL, G. H. Lander, J. M. Carpenter, R. L. Kustom, and T. K. Khoe, ICANS-VII Meeting, CRNL, September 13-16, 1983, CRNL Report [IN PRESS].

Accelerator System

Rapid Cycling Synchrotron (RCS) Single Stage Kicker Magnet, D. E. Suddeth and G. J. Volk, IEEE Conf. Records of 14th Pulse Power Modulator Symp., Orlando, FL, 1980, pp. 289-291.

Improvements in the Rapid Cycling Synchrotron, C. W. Potts, Proc. 5th Int. Collaboration Advanced Neutron Sources, June 1981, pp. 53-62.

Shaped Excitation Current for Synchrotron Magnets, M. H. Foss and W. Praeg, IEEE Trans. Nucl. Sci., NS-28 (1981), pp. 2856-2858.

Phase Lock of Rapid Cycling Synchrotron and Neutron Choppers, W. Praeg, D. McGhee, and G. Volk, IEEE Trans. Nucl. Sci., NS-28 (1981), p. 2171.

A Conceptual Design for an Accelerator System for a Very High-Intensity Pulsed Neutron Source using a Linear Induction Accelerator, M. H. Foss, IEEE Trans. Nucl. Sci., NS-28 (1981), pp. 3181-3183.

Study of the RF Capture Process in the Argonne Rapid Cycling Synchrotron, Y. Cho, C. W. Potts, A. V. Rauchas, S. Shin, and H. Takeda, IEEE Trans. Nucl. Sci., NS-28 (1981), p. 3040.

Observations and Cure of Head-Tail Effect in the Argonne Rapid Cycling Synchrotron, Y. Cho and A. V. Rauchas, IEEE Trans. Nucl. Sci., NS-28 (1981), p. 2585.

Determination of Transverse Phase-Space and Momentum Error from Size Measurements along the 50 MeV H^- RCS Injection Line, Y. Cho, E. A. Crosbie, and H. Takeda, IEEE Trans. Nucl. Sci., NS-28 (1981), pp. 3046-3048.

Measurements of H^0 and H^+ Ion Yields during H^- Acceleration in a 50 MeV Linac, Y. Cho, J. Madsen,

S. Shin, and V. Stipp, IEEE Trans. Nucl. Sci., NS-28 (1981), p. 2888.

An Intense H⁻ Source for the IPNS-I Rapid Cycling Synchrotron, D. R. Moffett and R. L. Barner, IEEE Trans. Nucl. Sci., NS-28 (1981), pp. 2678-2680.

Tune Control Improvements on the Rapid Cycling Synchrotron, C. W. Potts, M. Faber, G. Gunderson, M. J. Knott, and D. Voss, IEEE Trans. Nucl. Sci., NS-28 (1981), p. 3020.

Status Report on the Rapid Cycling Synchrotron, C. W. Potts, F. R. Brumwell, Y. Cho, A. V. Rauchas, and G. J. Volk, IEEE Trans. Nucl. Sci., NS-28 (1981), pp. 2104-2106.

The Rapid Cycling Synchrotron Extraction Kicker Magnet Drive System, D. E. Suddeth and G. J. Volk, IEEE Trans. Nucl. Sci., NS-28 (1981), pp. 3017-3019.

Betatron Tune Measurement at the Argonne Rapid Cycling Synchrotron, A. V. Rauchas, F. R. Brumwell, Y. Cho, W. S. Czyz, G. R. Gunderson, M. J. Knott, D. E. Suddeth, and G. J. Volk, IEEE Trans. Nucl. Sci., NS-28 (1981), p. 2331.

Beam Position Measurement System at the Argonne Rapid Cycling Synchrotron, A. V. Rauchas, F. R. Brumwell, Y. Cho, and W. S. Czyz, IEEE Trans. Nucl. Sci., NS-28 (1981), p. 2338.

Intense Pulsed Neutron Source, R. L. Kustom, IEEE Trans. Nucl. Sci., NS-28 (1981), pp. 3115-3119.

A Brighter H⁻ Source for the Intense Pulsed Neutron Source Accelerator System, V. Stipp, A. DeWitt, and J. Madsen, IEEE Trans. Nucl. Sci., NS-30 (1983), pp. 2743-2745.

Injected Beam Chopper System for the Intense Pulsed Neutron Source Accelerator System, A. Rauchas and R. Zolecki, IEEE Trans. Nucl. Sci., NS-30 (1983), pp. 2947-2949.

Performance of the Intense Pulsed Neutron Source Accelerator System, C. Potts, F. Brumwell, A. Rauchas, V. Stipp, and G. Volk, IEEE Trans. Nucl. Sci., NS-30 (1983), pp. 2131-2133.

A Proposed Second Harmonic Acceleration System for the Intense Pulsed Neutron Source Rapid Cycling Synchrotron, J. Norem, F. Brandeberry, and A. Rauchas, IEEE Trans. Nucl. Sci., NS-30 (1983), pp. 3490-3492.

IPNS Accelerator System and Neutron Chopper Synchronization, A. Rauchas, G. Ostrowski, C. Pelizzari, and G. Volk, ICANS-VII Meeting, CRNL, September 13-16, 1983, CRNL Report [IN PRESS].

Preliminary Tests of a Second Harmonic rf System for the Intense Pulsed Neutron Source Synchrotron, J. Norem and F. Brandeberry, ICANS-VII Meeting, CRNL, September 13-16, 1983, CRNL Report [IN PRESS].

Intense Pulsed Neutron Source Accelerator Status, C. W. Potts, F. R. Brumwell, and V. F. Stipp, ICANS-VII Meeting, CRNL, September 13-16, 1983, CRNL Report [IN PRESS].

Operating Experience with the IPNS Neutron Generating System, A. W. Schulke, D. E. Bohringer, B. S. Brown, and J. M. Carpenter, ICANS-VII Meeting, CRNL, September 13-16, 1983, CRNL Report [IN PRESS].

Targets and Moderators

Thermal Analysis of a Uranium Target Disc for Intense Pulsed Neutron Sources, J. L. Bailey, ANL Report ANL/ENG-81-06 (July 1981).

Design, Production, and Evaluation of a Zircaloy-Clad Uranium Target for an Intense Pulsed Neutron Source Application, B. A. Loomis, H. R. Thresh, G. L. Fogle, and S. B. Gerber, Nucl. Tech., 55 (1981), pp. 617-627.

The Liquid Hydrogen Moderator on the ZING-P′ Pulsed Spallation Neutron Source, J. M. Carpenter, R. Kleb, T. A. Postol, R. H. Stefiuk, and D. F. R. Mildner, Nucl. Instrum. Meth., 189 (1981), pp. 485-501.

Calculations of the Heat Deposition and the Expected Rate of Temperature Rise in Moderator, Reflector, and Decoupler Materials for IPNS-I, M. Kimura, J. M. Carpenter, and D. F. R. Mildner, ANL Report ANL-81-22 (1981).

Measurements of the Heat Deposition in Moderator and Decouplers in the ZING-P' Pulsed Spallation Neutron Source, J. M. Carpenter, M. Kimura, R. Kleb, M. Misawa, R. H. Stefiuk, and D. F. R. Mildner, Nucl. Instrum. Meth., 198 (1982), pp. 447-454.

Grooved Cold Moderator Tests, K. Inoue, Y. Kiyanagi, H. Iwasa, N. Watanabe, S. Ikeda, J. M. Carpenter, and Y. Ishikawa, ICANS-VI Meeting, ANL, June 27-July 2, 1982, ANL Report ANL-82-80 (1983), pp. 391-405.

An Evaluation of Structural Integrity of IPNS-I and ZING-P' Targets, J. M. Carpenter, H. Ahmed, B. Loomis, J. Ball, T. Ewing, J. Bailey, and A. F. D'Souza, ANL Report ANL-83-14 (1983).

Measurement and Fitting of Spectrum and Pulse Shapes of a Liquid Methane Moderator at IPNS, J. M. Carpenter, R. A. Robinson, and A. D. Taylor, ICANS-VII Meeting, CRNL, September 13-16, 1983, CRNL Report [IN PRESS].

Data Acquisition

The Data Acquisition System for the Neutron Scattering Instruments at the Intense Pulsed Neutron Source, R. K. Crawford, R. T. Daly, J. R. Haumann, R. L. Hitterman, C. B. Morgan, G. E. Ostrowski, and T. G. Worlton, IEEE Trans. Nucl. Sci., NS-28 (1981), pp. 3692-3700.

IPNS Distributed Processing Data Acquisition System, J. R. Haumann, R. T. Daly, T. G. Worlton, and R. K. Crawford, IEEE Trans. Nucl. Sci., NS-29 (1982), pp. 62-66.

The IPNS Data Acquisition System, T. G. Worlton, R. K. Crawford, J. R. Haumann, and R. Daly, ICANS-VI Meeting, ANL, June 27-July 2, 1982, ANL Report ANL-82-80 (1983), pp. 247-264.

Diffractometers and Spectrometers

High Resolution Powder Diffraction at the ZING-P' and IPNS-I Pulsed Neutron Sources, J. D. Jorgensen and F. J. Rotella, XIIth Congress and General Assembly, Int. Union Cryst., Ottawa, Canada, 16-25 August, 1981 [ABSTRACT].

Tests of a Resonance Detector Spectrometer, J. M. Carpenter, N. Watanabe, S. Ikeda, Y. Masuda, and S. Sato, KENS Report III, A Report of Japanese Lab. for High Energy Physics, Tsukuba, Japan, KEK Internal Report, July 1982.

Tests of a Resonance Detector Spectrometer for Electron-Volt Spectroscopy, J. M. Carpenter, N. Watanabe, S. Ikeda, Y. Masuda, and S. Sato, ICANS-VI Meeting, ANL, June 27-July 2, 1982, ANL Report ANL-82-80 (1983), pp. 265-277.

A Resonance Detector Spectrometer at KENS, J. M. Carpenter, N. Watanabe, S. Ikeda, Y. Masuda, and S. Sato, Physica, 120B (1983), pp. 126-130.

Time Focussing and Resolution in Resonance Detector Neutron Spectrometers, J. M. Carpenter and N. Watanabe, Nucl. Instrum. Meth., 213 (1983), pp. 311-316.

Small Angle Scattering Diffractometer Developed for Metallurgical Type Application at the Argonne Pulsed Neutron Source, IPNS-I', J. E. Epperson and C. S. Borso, Am. Cryst. Assoc. Meeting, August 1982 [ABSTRACT].

Small Angle Scattering at a Pulsed Neutron Source: Comparison with a Steady State Reactor, C. S. Borso, J. M. Carpenter, F. S. Williamson, G. L. Holmblad, M. H. Mueller, J. Faber, Jr., J. E. Epperson, and S. S. Danyluk, J. Appl. Cryst., 15 (1982), pp. 443-448.

The Spin Precession Resonance Spectrometer, G. P. Felcher and J. M. Carpenter, Nucl. Instrum. Meth., 192 (1982), pp. 513-522.

Collection and Analysis of Single Crystal Time-of-Flight Data at Argonne's Pulsed Neutron Source, A. J. Schultz, R. G. Teller, S. W. Peterson, and J. M. Williams, in **Neutron Scattering - 1981**, J. Faber, Jr. (Ed.), Am. Inst. Phys. Conf. Proc., 89 (1982), pp. 35-41.

High Resolution Time-of-Flight Powder Diffractometer at the ZING-P' Pulsed Neutron Source, J. D. Jorgensen and F. J. Rotella, J. Appl. Cryst., 15 (1982), pp. 27-34.

Single Crystal Time-of-Flight Neutron Diffraction at IPNS, A. J. Schultz, P. Leung, and J. M. Williams, Am. Chem. Soc., 185th ACS Nat. Meeting, Seattle, WA, March 20-25, 1983, INOR-3 [ABSTRACT].

High Resolution Powder Diffraction and Rietveld Analysis at Pulsed Neutron Sources, J. D. Jorgensen, Am. Chem. Soc., 185th ACS Nat. Meeting, Seattle, WA, March 20-25, 1983 [ABSTRACT].

Recent Results on the General Purpose Powder Diffractometer at Argonne's Pulsed Neutron Source, J. Faber, Jr., Am. Chem. Soc., 185th ACS Nat. Meeting, Seattle, WA, March 20-25, 1983 [ABSTRACT].

The IPNS Time-of-Flight Single Crystal Diffractometer, A. J. Schultz, R. G. Teller, and J. M. Williams, ICANS-VI Meeting, ANL, June 27-July 2, 1982, ANL Report ANL-82-80 (1983), pp. 115-124.

The IPNS-I Chopper Spectrometers, D. L. Price, J. M. Carpenter, C. A. Pelizzari, S. K. Sinha, I. Bresof, and G. E. Ostrowski, ICANS-VI Meeting, ANL, June 27-July 2, 1982, ANL Report ANL-82-80 (1983), pp. 207-215.

Electronically Focused Powder Diffractometers at IPNS-I, J. D. Jorgensen and J. Faber, ICANS-VI Meeting, ANL, June 27-July 2, 1982, ANL Report ANL-82-80 (1983), pp. 105-114.

Time of Flight Spectrometer for Ultra-Cold Neutrons, J. W. Lynn, W. A. Miller, T. W. Dombeck, G. R. Ringo, V. E. Krohn, and M. S. Freedman, Physica, 120B (1983), p. 114.

Instrumentation at Pulsed Neutron Sources, J. M. Carpenter, G. H. Lander, and C. G. Windsor, Rev. Sci. Instrum. [IN PRESS].

CONDENSED MATTER RESEARCH

Crystalline

Sn and Fe Sites in $SnFe_{0.4}Mo_6S_8$. A Powder Neutron Diffraction Study, J. D. Jorgensen, D. G. Hinks, and F. J. Rotello, in **Ternary Superconductors**, Elsevier North Holland, 1981, pp. 69-73.

Fe Defect Sites in $YbFe_xMo_6S_8$, J. D. Jorgensen, D. G. Hinks, F. J. Rotella, G. K. Shenoy, and D. R. Noakes, Bulletin Am. Phys. Soc., 27 (1982), p. 320 [ABSTRACT].

Neutron Powder Diffraction of Forsterite, Mg_2SiO_4: A Comparison with Single-Crystal Investigations, A. Lager, F. K. Ross, F. J. Rotella, and J. D. Jorgensen, J. Appl. Cryst., 14 (1981), pp. 137-139.

Structural Studies of Precursor and Partially Oxidized Conducting Complexes. 21 Single Crystal and Powder Time-of-Flight Neutron Diffrcction Studies of $Tl_4[Pt(CN)_4]CO_3$, M. A. Beno, F. J Rotella, J. D. Jorgensen, and J. M. Williams, Inorg. Chem., 20 (1981), pp. 1802-1806.

Conduction Plane and Structure of Li-Stabilized Na β''-Alumina: A Powder Neutron Diffraction Study, J. D. Jorgensen, F. J. Rotella, and W. L. Roth, Solid State Ionics, 5 (1981), pp. 143-146.

Neutron Powder Diffraction Study of Defect Spinel Structures: Tetrahedrally-coordinated Ti^{4+} in $Ni_{2.62}Ti_{0.69}O_4$ and $Ni_{2.42}Ti_{0.74}Si_{0.05}O_4$, G. A. Lager, T. Armbruster, F. K. Ross, F. J. Rotella, and J. D. Jorgensen, J. Appl. Cryst., 14 (1981), pp. 261-264.

Powder Diffraction Study of Phase Transitions in the Spinel $NiCr_2O_4$, T. Armbruster, G. A. Lager, J. Ihringer, F. J. Rotella, and J. D. Jorgensen, Am. Cryst. Assoc. Winter Meeting, Columbia, MO, March 1983, p. 33 [ABSTRACT].

Neutron and X-ray Powder Study of Phase Transitions in the Spinel $NiCr_2O_4$, T. Armbruster, G. A. Lager, J. Ihringer, F. J. Rotella, and J. D. Jorgensen, Z. Kristallogr., 162 (1983), p. 8.

Location of Deuterium Sites in $DTaWO_6$ from Neutron Powder Data, F. J. Rotella, J. D. Jorgensen, G. A. Lager, and F. K. Ross, Programs and Abstracts, Am. Cryst. Assoc., 1981, p. 23 [ABSTRACT].

Deuterium Sites in the Defect Pyrochlore $DTaWO_6$: Location from Neutron Powder Diffraction Data, F. J. Rotella, J. D. Jorgensen, B. Morosin, and R. M. Biefeld, Solid State Ionics, 5 (1981), pp. 455-458.

Location of Deuterium Sites in the Defect Pyrochlore $DTaWO_6$ from Neutron Powder Diffraction Data, F. J. Rotella and J. D. Jorgensen, Acta Cryst., B38 (1982), pp. 1697-1703.

Neutron Diffraction Investigation of Ordered Oxygen Vacancies in $Pb_2Ru_2O_{6.5}$, R. A. Beyerlein, H. S. Horowitz, J. M. Longo, J. D. Jorgensen, and F. J. Rotella, in **Neutron Scattering - 1981**, J. Faber, Jr. (Ed.), Am. Inst. Phys. Conf. Proc., 89 (1982), pp. 78-80.

Diffraction Studies of Cemented Carbide Composites Using the Argonne Intense Pulsed Neutron Source, A. D. Krawitz and J. Faber, J. Met., 35 (1982), p. 11.

A Search for the "True" Boehmite, δ-AlOOH. X-Ray and Neutron Powder Diffraction Structure Determination, C. E. Corbato, R. T. Tettenhorst, J. M. Williams, F. J. Rotella, J. D. Jorgensen, and G. G. Christoph, Abstracts and Papers, Am. Cryst. Assoc. Winter Meeting, March 29-April 2, 1982, Abstract H4-17, No. 14, p. 27 [ABSTRACT].

Neutron Diffraction Studies of $CeVO_4$, $PrVO_4$ and $ScVO_4$, J. Faber and A. T. Aldred, in **Neutron Scattering - 1981**, J. Faber, Jr. (Ed.), Am. Inst. Phys. Conf. Proc., 89 (1982), pp. 72-74.

Nonstoichiometry in the Chevrel-Phase Compounds Sn and $PbMo_6S_8$, D. G. Hinks, J. D. Jorgensen, G. W. Crabtree, and H-C. Li, Bulletin Am. Phys. Soc., 27 (1982), pp. 318-319 [ABSTRACT].

Defects in Chevrel-Phase Structures, J. D. Jorgensen and D. G. Hinks, Program and Abstracts, Am. Cryst. Assoc. Winter Meeting, Columbia, MO, March 14-18, 1983, p. 25.

Valence and Delocalization of Yb in the Chevrel-Phase $YbMo_6S_8$, J. D. Jorgensen, D. G. Hinks, D. R. Noakes, P. J. Viccaro, and G. K. Shenoy, Phys. Rev., B27 (1983), pp. 1465-1473.

The Nature of the Oxygen-Containing Defect in Chevrel-Phase Materials, D. G. Hinks, J. D. Jorgensen, and H-C. Li, Bulletin Am. Phys. Soc., 28 (1983), p. 301 [ABSTRACT].

Delocalization and Thermal Expansion in Chevrel-Phase Structures, J. D. Jorgensen and D. G. Hinks, Bulletin Am. Phys. Soc., 28 (1983), p. 301 [ABSTRACT].

Oxygen Impurity in the Chevrel-Phase $SnMo_6S_8$, D. G. Hinks, J. D. Jorgensen, and H-C. Li, Solid State Commun. [IN PRESS].

The Structural Characterization of the C-H-Metal Interaction in $Mn(CO)_3(C_7H_{11})$ Using Pulsed Neutron Time-of-Flight Data, A. J. Schultz, R. G. Teller, M. A. Beno, and J. M. Williams, Abstracts and Papers, 184th ACS Nat. Meeting, Kansas City, MO, September 12-17, 1982, INOR-98 [ABSTRACT].

Interstitial Site Occupation in ZrNiH, D. G. Westlake, H. Shaked, P. R. Mason, B. R. McCart, M. H. Mueller, T. Matsumoto, and M. Amano, J. Less-Common Met., 88 (1982), pp. 17-23.

Distribution of Hydrogen Vibrations in $LaH_{2.28}$ and $LaH_{2.99}$, W. A. Kamitakahara and R. K. Crawford, Solid State Commun., 41 (11) (1982), pp. 843-847.

Crystal Structure and Thermal Expansion of α-SiO_2 at Low Temperatures, G. A. Lager, J. D. Jorgensen, and F. J. Rotella, **Neutron Scattering - 1981**, J. Faber, Jr. (Ed.), Am. Inst. Phys. Conf. Proc., 89 (1982), pp. 75-77.

Crystal Structure and Thermal Expansion of α-Quartz SiO_2 at Low Temperatures, G. A. Lager, J. D. Jorgensen, and F. J. Rotella, J. Appl. Phys., 53 (1982), pp. 6751-6756.

The Use of Time-of-Flight Neutron Diffraction to Study Grain Interaction Stresses, S. R. MacEwen, J. Faber, and A. P. L. Turner, Acta Metallurg., 31 (1983), pp. 657-676.

Neutron Powder Diffraction Studies in the System $CaSO_4 \cdot H_2O$, G. A. Lager, T. Armbruster, F. J. Rotella,

J. D. Jorgensen, and D. G. Hinks, Z. Kristallogr., 162 (1983), p. 160.

A Crystallographic Study of the Low-Temperature Dehydration Products of Gypsum, $CaSO_4 \cdot 2H_2O$: Hemihydrate, $CaSO_4 \cdot 0.5H_2O$, and γ-$CaSO_4$, G. A. Lager, T. Armbruster, F. J. Rotella, J. D. Jorgensen, and D. G. Hinks, Am. Mineral. [IN PRESS].

Studies of Zeolitic Materials using Neutron Powder Diffraction, J. B. Parise, E. Prince, D. E. Cox, and J. D. Jorgensen, Am. Cryst. Assoc. Winter Meeting, Columbia, MO, March 14-18, 1983, p. 26 [ABSTRACT].

Neutron Diffraction Studies of C-H Bond Activation, A. J. Schultz and J. M. Williams, Programs and Abstracts, Am. Cryst. Assoc. Winter Meeting, Columbia, MO, March 14-18, 1983, Vol. II, No. 1, Abstract J2, p. 22 [ABSTRACT].

Deuterium Site Preference in the Oxygen-Stabilized η-Carbide $Zr_3V_3OD_x$ - A Neutron Powder Diffraction Study, F. J. Rotella, H. E. Flotow, D. M. Gruen, D. G. Westlake, and J. D. Jorgensen, Am. Cryst. Assoc. Winter Meeting, Columbia, MO, March 14-18, 1983, p. 22 [ABSTRACT].

Deuterium Site Occupation in the Oxygen-Stabilized η-Carbides $Zr_3V_3OD_x$: I. Preparation and Neutron Powder Diffraction, F. J. Rotella, H. E. Flotow, D. M. Gruen, and J. D. Jorgensen, J. Chem. Phys. [IN PRESS].

Argonne Intense Neutron Source used to Solve the Molecular Structure of a Novel Organometallic Complex, A. J. Schultz, R. G. Teller, M. A. Beno, J. M. Williams, M. Brookhart, W. Lamanna, and M. B. Humphrey, Science, 220 (April 1983), pp. 197-199.

A New Oxygen-Deficient Manganese Perovskite, $CaMnO_{2.75}$, R. A. Beyerlein, J. M. Longo, M. E. Leonowicz, and J. D. Jorgensen, Fall Meeting, ACS, Kansas City, MO, September 12-17, 1983 [ABSTRACT].

Crystal Structure Studies on Yttria Stabilized Zirconia at High Temperatures Using Pulsed Neutron Single Crystal Diffractometer, H. Horiuchi, A. J. Schultz, P. Leung, and J. M. Williams, Abstracts, Japanese Cryst. Assoc. Meeting, Sendai, November 14-16, 1983.

Single Crystal Time-of-Flight Neutron Diffraction Structure of $[cis\text{-}(OC)_4Re(CH_3CO)_2]H$: A Metallaacetylacetone Molecule, A. J. Schultz, K. Srinivasan, R. G. Teller, J. M. Williams, and C. M. Lukehart, J. Am. Chem. Soc. [IN PRESS].

Magnetic Structures

Structural and Magnetic Studies of Hexagonal β-$^{242}Pu_2O_3$, B. McCart, G. H. Lander, and A. T. Aldred, J. Chem. Phys., 74 (1981), pp. 5263-5268.

Neutron Scattering Experiments on CeB_6, M. Loewenhaupt, and J. M. Carpenter, Bulletin Am. Phys. Soc., 28 (1983), p. 286 [ABSTRACT].

Magnetic Moments in $PrCo_5$, S. Rinaldi, F. Leccabue, G. P. Felcher, and J. D. Jorgensen, Bulletin Am. Phys. Soc., 28 (1983), p. 367 [ABSTRACT].

Magnetic Response of Spin Fluctuation System UAl_2, M. Loewenhaupt and C-K. Loong, Bulletin Am. Phys. Soc., 28 (1983), p. 341 [ABSTRACT].

Neutron Scattering Investigation of the Magnetic Ground State of PrO_2, S. Kern, C-K. Loong, J. Faber, Jr., and G. H. Lander, Solid State Commun. [IN PRESS].

Magnetic Structures of Monoclinic FeGe, G. P. Felcher, J. D. Jorgensen, and R. Wappling, J. Phys. C, 16 (1983) [IN PRESS].

Neutron Scattering Study of the Magnetic Excitations in Ferromagnetic Iron at High Energy Transfers, C-K. Loong, J. M. Carpenter, J. W. Lynn, R. Robinson, and H. A. Mook, J. Appl. Phys. [IN PRESS].

Battery and Electrodes

Structural and Dynamical Properties of Defects in the Battery Electrode β-LiAl, at Elevated Temperatures, T. O. Brun and S. Susman, Bulletin Am. Phys. Soc., 27 (1982), pp. 351-352 [ABSTRACT].

Microscopic Properties of the Mixed-Conducting Electrode β-LiAℓ. T. O. Brun, Bulletin Am. Phys. Soc., 27 (1982), p. 351 [ABSTRACT].

Defects and Disorder in the Fast-Ion Electrode Lithium-Aluminum, T. O. Brun, J. D. Jorgensen, M. Misawa, F. J. Rotella, S. Susman, and D. F. R. Mildner, J. Electrochem. Soc., 129 (1982), pp. 2509-2512.

Lead Deficiency and Hydrogen Content in Battery Electrode β-PbO$_2$, J. D. Jorgensen, R. Varma, F. J. Rotella, G. Cook, and N. P. Yao, J. Electrochem. Soc., 129 (1982), pp. 1678-1681.

Hydrogen Content and Lead Vacancies in β-PbO$_2$ from Active Battery Plates, J. D. Jorgensen, R. Varma, F. J. Rotella, G. Cook, and N. P. Yao, in **Neutron Scattering - 1981**, John Faber, Jr. (Ed.), Am. Inst. Phys. Conf. Proc., 89 (1982), pp. 81-83

Amorphous Materials

The Short-Range Structure of Alkali Disilicate Glasses by Pulsed Neutron Total Scattering, M. Misawa, D. L. Price, and K. Suzuki, J. Non-Crystall. Solids, 37 (1980), pp. 85-97.

On the Short Range Atomic Structure of Non-Crystalline Carbon, J. M. Carpenter and D. F. R. Mildner, J. Non-Crystall. Solids, 47 (1982), pp. 391-401.

Mixing of Phases in Non-Crystalline Materials: Application to Carbon, G. C. Summerfield, D. F. R. Mildner, and J. M. Carpenter, J. Non-Crystall. Solids, 57 (1983), pp. 289-303.

Structures of Selenium/Phosphorus Glasses, D. L. Price and S. Susman, Bulletin Am. Phys. Soc., 27 (3) (March 1982), p. 178 [ABSTRACT].

Neutron Scattering Measurement of the Dynamical Structure Factor of Amorphous SiO$_2$, J. M. Carpenter, D. L. Price, and C. A. Pelizzari, Bulletin Am. Phys. Soc., 28 (1983), p. 455 [ABSTRACT].

The Structure of Phosphorus - Selenium Glasses I. Concentration Dependence of the Short- and Intermediate-Range Order, D. L. Price, M. Misawa, S. Susman, T. I. Morrison, G. K. Shenoy, and M. Grimsditch, J. Non-Crystall. Solids [IN PRESS].

Quantum Solids

Spin Structure of Solid ^{3}He below 1 mK by Neutron Diffraction, P. R. Roach, S. K. Sinha, B. K. Sarma, M. Vrtis, Y. Takano, M. Misawa, K. Sköld, R. Kleb, Z. Sungaila, J. B. Ketterson, and W. P. Halperin, Symp. Quantum Fluids and Solids, Sanibel, FL, April 11-15, 1983.

Neutron Diffraction from Solid ^{3}He, P. R. Roach, S. K. Sinha, Z. Sungaila, R. Kleb, Y. Takano, M. Misawa, B. K. Sarma, M. Vrtis, W. P. Halperin, J. B. Ketterson, and K. Sköld, Am. Phys. Soc. Meeting, Baltimore, MD, April 18-22, 1983.

Use of an Intense Pulsed Neutron Source to Measure Momentum Density in Condensed Phase, R. O. Hilleke, P. Chaddah, R. O. Simmons, D. L. Price, and S. K. Sinha, Bulletin Am. Phys. Soc., 28 (1983), p. 291 [ABSTRACT].

RADIATION EFFECTS FACILITY AND RESEARCH

Measurements of Neutron Spectra and Fluxes at Spallation-Neutron Sources and their Application to Radiation Effects Research, M. A. Kirk, R. C. Birtcher, T. H. Blewitt, L. R. Greenwood, and R. R. Heinrich, J. Nucl. Mater., 96 (1981), pp. 37-50.

Radiation Effects in Superconducting Fusion-Magnet Materials, B. S. Brown, J. Nucl. Mater., 97 (1981), pp. 1-14.

Critical Current Changes in NbTi during Fast-Neutron Irradiation at 6 K, R. C. Birtcher, B. S. Brown, and T. L. Scott, J. Nucl. Mater., 97 (1981), pp. 337-338.

Neutron Irradiation Facilities at the Intense Pulsed Neutron Source-I, B. S. Brown and T. H. Blewitt, J. Nucl. Mater., 103/104 (1981), pp. 1567-1572.

Neutron Irradiation Facilities at the Intense Pulsed Neutron Source-I for Fusion-Magnet Materials Studies, B. S. Brown and T. H. Blewitt, Proc. Fast, Thermal and Fusion Reactor Experiments Conf., Salt Lake City, Utah, April 12-15, 1982, Vol. II, pp. 2-235 to 2-245.

Neutron Irradiation Facilities at the Intense Pulsed Neutron Source, R. C. Birtcher, T. H. Blewitt, M. A. Kirk, T. L. Scott, B. S. Brown and L. R. Greenwood, J. Nucl. Mater., 108/109 (1982), pp. 3-9.

Spallation Neutron Damage in Group IV, III-V and II-VI Semiconductors at 5 K, R. C. Birtcher, J. M. Meese, and T. L. Scott, 4th Neutron Transmutation Doping Conf., Washington, DC, June 1, 1982.

Spallation and 14 MeV Neutron Irradiation of Stabilized NbTi Superconductors, P. Hahn, B. S. Brown, H. W. Weber, and M. W. Guinan, Int. Cryogenic Materials Conf., Colorado Springs, August 15-19, 1983.

Observations of In-Situ Tensile Deformation and Fracture in Neutron Irradiated Niobium in an HVEM, B. A. Loomis and M. P. Otero, 3rd Top. Meeting on Fusion Reactor Materials, Albuquerque, NM, September 19-22, 1983 [ABSTRACT].

A Comparison of Fission Neutron and Pulsed Spallation Neutron Sources for Radiation Effects Experiments on Cu_3Au, M. A. Kirk, Int. Symp. Use and Development of Low and Medium Flux Research Reactors, MIT, Cambridge, MA, October 17-19, 1983 [ABSTRACT].

Radiation Effects of the Intense Pulsed Neutron Source at Argonne National Laboratory, R. C. Birtcher and T. L. Scott, Int. Symp. Use and Development of Low and Medium Flux Research Reactors, MIT, Cambridge, MA, October 17-19, 1983 [ABSTRACT].

Methods of Neutron and Proton Dosimetry at Spallation Sources, L. R. Greenwood and R. J. Popek, ICANS-VI Meeting, ANL, June 27-July 2, 1982, ANL Report ANL-82-80 (1983), pp. 605-617.

Measurement of Neutron Spectra and Fluxes at the IPNS Radiation Effects Facility, R. C. Birtcher, M. A. Kirk, T. H. Blewitt, and L. R. Greenwood, ICANS-VI Meeting, ANL, June 27-July 2, 1982, ANL Report ANL-82-80 (1983), pp. 407-429.

Point Defect Production and Annihilation in Neutron-Irradiated Zr, S. R. MacEwen, R. H. Zee, and R. C. Birtcher, J. Nucl. Mater. [IN PRESS].

Radiation Damage Studies, M. Kirk, ICANS-VII Meeting, CRNL, September 13-16, 1983, CRNL Report [IN PRESS].

Irradiation Effects on the Mechanical Properties of Composite Organic Insulators, S. Egusa, M. A. Kirk, R. C. Birtcher, M. Hagiwara, and S. Kawanishi, Radiation Effects [IN PRESS].

THEORY AND TECHNIQUES

General

Neutron Reflection as a Probe of Surface Magnetism, G. P. Felcher, Phys. Rev., B24 (1981), pp. 1595-1598.

Neutron Probes, D. L. Price, Popular Science Magazine, 219 (2) (1981), pp. 55-57.

Neutron Guide Tube Gain for a Remote Finite Source, J. M. Carpenter and D. F. R. Mildner, Nucl. Instrum. Meth., 198 (1981), pp. 341-348.

Power Densities in Materials in Spallation Neutron Source Environments, M. Kimura, J. M. Carpenter, and D. F. R. Mildner, Nucl. Instrum. Meth., 198 (1982), pp. 433-445.

Rietveld Refinement with Spallation Neutron Powder Diffraction Data, R. B. von Dreele, J. D. Jorgensen, and C. G. Windsor, J. Appl. Cryst., 15 (1982), pp. 581-589.

Some Optimization Considerations in Chopper Inelastic Neutron Scattering Experiments, M. Kimura, C. A. Pelizzari, and J. M. Carpenter, Nucl. Instrum. Meth., 203 (1982), pp. 537-545.

Empirical Collection of Wavelength-Dependent Extinction Effects in Neutron Diffraction, P. C. W. Leung, A. J. Schultz, J. M. Williams, and R. A. Jacobson, Program and Abstracts, Am. Cryst. Assoc. Winter Meeting, Columbia, MO, March 14-18, 1983, Abstract PC11, p. 35 [ABSTRACT].

Simulated Time-of-Flight Neutron Powder Diffraction Data-Generation and Uses, F. J. Rotella and T. M. Sabine, Program and Abstracts, 32nd Ann. Denver

X-ray Conf. and Am. Cryst. Assoc. Combined Meeting, Snowmass, CO, August 1-5, 1983, p. 51 [ABSTRACT].

Utilization of the IPNS at Argonne National Laboratory for Neutron Activation Analysis, R. R. Heinrich, L. R. Greenwood, R. J. Popek, and A. W. Schulke, 26th ORNL-DOE Conf. Analytical Chem. in Energy Technology, Knoxville, TN, October 11-13, 1983.

A New Probe for Surface Magnetism: Polarized Neutron Reflection, S. D. Bader, G. P. Felcher, K. E. Gray, and R. T. Kampwirth, Physica, 120B (1983), p. 219 [ABSTRACT].

Polarized Neutron Techniques and Applications, G. P. Felcher, ICANS-VI Meeting, ANL, June 27-July 2, 1982, ANL Report ANL-82-80 (1983), p. 179 [ABSTRACT].

A Rotating Crystal Pulse Shaper for Use in a Pulsed Neutron Source, J. M. Carpenter and C. J. Carlile, ICANS-VI Meeting, ANL, June 27-July 2, 1982, ANL Report ANL-82-80 (1983), pp. 217-235.

A Rotating-Crystal Pulse Shaper for Use on a Pulsed Neutron Source, J. M. Carpenter and C. J. Carlile, J. Appl. Cryst., 16 (1983), pp. 363-369.

Tests of the Spin Refrigerator as a Neutron Spin Filter, G. P. Felcher, R. Kleb, D. G. Hinks, and W. H. Potter, Bulletin Am. Phys. Soc., 28 (1983), p. 286 [ABSTRACT].

Position Sensitive Detectors

New Position-Sensitive Neutron Detector, M. G. Strauss, R. Brenner, and F. J Lynch, Program and Abstracts, 5th Int. Conf. Small Angle Scattering, Berlin, West Germany, October 1980, p. 206 [ABSTRACT].

Requirements of Position-Sensitive Detectors for Neutron Scattering Experiments, R. K. Crawford and J. M. Carpenter, IEEE Trans. Nucl. Sci., NS-28 (1981), pp. 792-799.

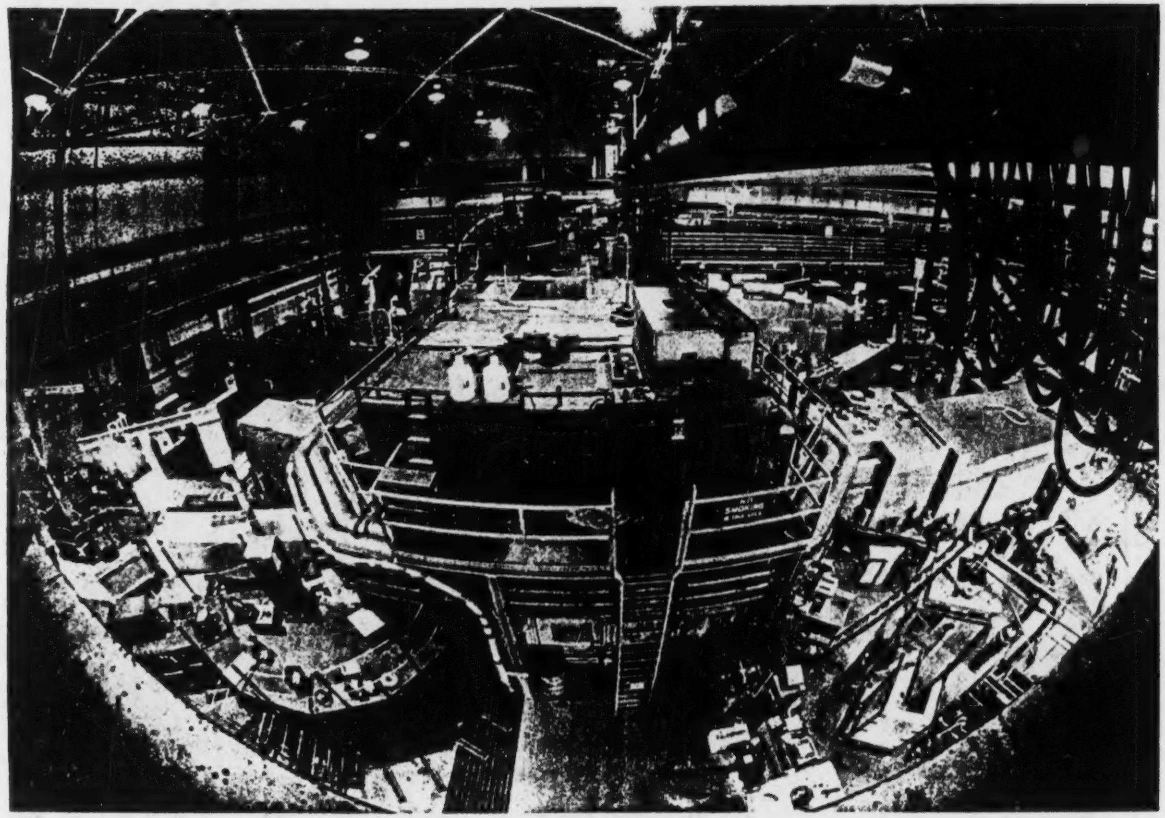
2-D Position-Sensitive Scintillation Detector for Neutrons, M. G. Strauss, R. Brenner, F. J. Lynch, and C. B. Morgan, IEEE Trans. Nucl. Sci., NS-28 (1981), p. 800.

Summary of Position-Sensitive Detector Workshop, G. H. Lander and R. Allemand, Workshop on Position-Sensitive Detection of Thermal Neutrons, Institut Laue Langevin, Grenoble, France, October 11-12, 1982, Academic Press [IN PRESS].

Spatial Resolution of Neutron-Position Scintillation Detectors, M. G. Strauss, R. Brenner, H. P. Chou, A. J. Schultz, and C. T. Roche, Workshop on Position-Sensitive Detection of Thermal Neutrons, Institut Laue Langevin, Grenoble, France, October 11-12, 1982, Academic Press [IN PRESS].

A 2-D Position-Sensitive Scintillation Neutron Detector for the Time-of-Flight Single-Crystal Diffractometer at IPNS, A. J. Schultz, R. G. Teller, J. M. Williams, M. G. Strauss, and R. Brenner, Trans. Am. Cryst. Assoc., 18 (1982), pp. 169-179.

Resonance Neutron Radiography using a Pulsed Neutron Source and a 2-Dimensional Scintillation Detector, M. G. Strauss, G. H. Lander, R. Brenner, and C. T. Roche, in **Neutron Radiography**, J. P. Barton and P. Von der Hardt (Eds.), Riedel Pub. Co., Dordrecht, Holland, 1983, pp. 519-530.



Wide-angle view of IPNS facility. The accelerator, which is not shown but is in the background, fires protons straight at the observer. They strike a uranium target and the neutron instruments can be seen around the central monolith, with path lengths extending out to 20 m.

2.5 Premium Coal Sample Program

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

   Answer: The Premium Coal Sample Program will make possible the conduct of a new level of basic research on the constitution, structure and reactivity of coal. Uniquely prepared and essentially identical samples provided by this program will provide the first opportunity for research people at different laboratories to correlate their work with that of other scientists using truly comparable samples. This marks a time for the coal chemist analogous to the first availability of reagent grade chemicals to the inorganic or organic chemist. The opportunity that will be exploited is the prospect of correlating the results of diverse studies to bring about a new depth of understanding about the constitution, structure, properties and reactivity of coals.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

   Answer: The uniqueness of this program lies in the complete enclosure of the processing train to provide minimal exposure to oxygen (to avoid any oxidative changes), and to control and maintain the humidity (to avoid changes to the pore structure within the coal). In addition a large blender provides uniform mixing of a large batch of pulverized coal. This blending contrasts with the usual riffling, which is a tedious, repetitive operation, and may subject the samples to the risk of oxygen exposure due to the long time and handling required. Statistical studies have demonstrated that thorough mixing is achieved via blending in a short time. The final samples are collected in glass ampoules which are flame sealed to provide a secure barrier to any inflow of oxygen or outflow of the humid nitrogen environment. The ampoules are made of amber glass to minimize photon-induced reactions. For each type of coal processed, 15,000 samples (5g and 20g sizes) will be prepared initially. Enough material will be held in reserve to provide 60,000 additional samples. Thus, a long-term supply of very high quality, well-characterized samples will be assured for study by the coal research community. Each coal will require about 3 weeks to process.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

   Answer: The principal objective of the Premium Coal Sample Program is the collection, preparation and distribution of well-characterized coal samples to the coal community. Most of the instrumentation associated with this program is focused on this objective. However, one large controlled-atmosphere glovebox which houses a Giesler plastometer is available for research on the stability of coal as a function of time, temperature and oxygen level.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

   Answer: The program was initiated in December of 1982. Construction of the facility is in progress and completion of the facility is expected by July, 1984. We anticipate that three different types of coal will be processed in FY84, another three in FY85 and two more are planned for processing in FY86.

By processing we mean the mining, pulverizing, and blending of a coal, and the packaging of identical samples in a large number of sealed glass ampoules for use by researchers.

5. What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?

Answer: This is a new facility and no changes or additions from the original plan are anticipated. The level and type of interest expressed by the research community will guide changes that may be made in the future.

6. For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).

Answer:

(Budget Authority In Thousands)

	FY81	FY82	FY83	FY84	FY85	Source of Funds
Facility Operation*	0	0	0	95	220	Chemical Sciences
In-House Research	0	0	0	0	100	Chemical Sciences
Out-of-House Research** (User Research Support)	0	0	0	0	3000	
Other Operating Expenses (Construction)	0	454	645	527	382	Chemical Sciences
Capital Equipment	0	0	150	81	20	Chemical Sciences

*The Facility will begin operation in July 1984.

**This entry in FY85 represents our estimate of the research support provided non-Argonne recipients of samples through their home institutions for work in which these samples play a prominent role.

7. How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?

Answer: To date no funding has been received from sources other than the DOE. Funding from other sources may be provided by organizations which request the processing of additional coals on a cost reimbursement basis. An Australian group has expressed interest in processing up to 4 brown coals at a cost of about $40,000 each.

8. For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.

Answer:

	FY81	FY82	FY83	FY84	FY85
Man Years (Facility Construction and Operation)	0	0	4.2	3.6	3.9

9. What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?

Answer: The facility will become operational in July 1984. By the end of FY 1985, six coal batches will have been processed. The processing of four additional coal batches for an Australian group is under negotiation. The facility has the capability to process 15 coal batches per year.

10. For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?

Answer: This is a new facility intended to prepare coals in a unique manner for distribution to the basic research community. The program began in December 1982, and calls for the processing of three coals in each of FY84 and FY85. This schedule is expected to be met.

11. What is this facility's user policy?

Answer: The user policy has several elements. Samples will be made available to all qualified basic research people. A nominal charge will be made for samples to defray replacement cost over a period of time. Sample recipients will be asked to provide references to published reports and other publications which may result from research on supplied samples, so that they may be shared with the rest of the basic research community. The facility will be made available to external sponsors for the processing of suitable coals on a reimbursed cost basis. The same standards used for the collection, preparation and distribution of samples for the Premium Coal Sample Program will apply to any externally sponsored efforts. Work for external sponsors will be done subject to the schedule for the work sponsored by the U. S. Department of Energy.

12. For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?

Answer:

(Budget Authority in Thousands)

	FY81	FY82	FY83	FY84	FY85
Reimbursable Research	0	0	0	0	$160*

*Revenue for the processing of four Australian coals

13. What is the mechanism by which specific research proposals for experiments at the facility are considered?

Answer: This facility processes coal for the use of the basic research community; it does not conduct research nor provide facilities for research on the samples prepared. Proposals for the processing of coals in the facility received from potential external sponsors will be reviewed initially by the Program Manager, then by the U. S. Department of Energy and finally by the Users Advisory Committee.

14. How many research proposals have been submitted over the past five years, and how many of these have been approved?

Answer: Because of its character, no proposals for research at this facility have been or will be received; however, 238 individuals have requested that their names be placed on a mailing list for sample availability announcements. The requests have come from highly respected sources, e.g., members of the Fuel Chemistry Division of the American Chemical Society, attendees of the July 1983 Gordon Research Conference on Fuel Science, attendees of the August 1983 International Conference on Fuel Science in Pittsburgh, and from a number of research laboratories in this country.

15. How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?

Answer: Seventy-two (72) requests have been received from university personnel contemplating the use of premium coal samples for their research.

16. How many industrial researchers have utilized the facility over the past five years?

Answer: Eighty-nine (89) requests for premium coal samples have been received from industry researchers and consultants involved in research in coal.

17. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer: There have been 38 requests for premium coal samples from foreign research workers. The requests originated from every inhabited continent except Africa.

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: None. ("Researchers from other agencies" are defined as regular employees of agencies, federal or state, other than DOE or GOCO contractors.) It should be noted that scientists from other DOE laboratories use this facility.

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: Future possibilities for this facility include the development of unique packaging methods for separated coal macerals (the individual constituents of coal organic matter), and the processing of coals and oil shale for external organizations. To handle coal macerals the processing facility will have to be modified.

20. Please provide a copy of the facility's latest annual report.

Answer: No formal reports on facility use are prepared, since this is not operated as a formal user facility. Reports of progress and accomplishment are prepared for DOE - Chemical Sciences in the Field Task Proposals and in an annual report, "Surveys of Research in the Chemistry Division" which is prepared for our Review Committees and for general interest. A copy of the relevant pages of the most recent "Surveys of Research in the Chemistry Division" is included.

IX. PREMIUM COAL SAMPLE PROGRAM (K. S. Vorres)

Outside Collaborators (J. Young, K. M. Myles)

The major purpose of the Premium Coal Sample Program is to provide the coal science community with long-term supplies of premium samples of a small number of coals that can be used as standards of comparison. The premium coal samples produced from each coal and distributed through this program will be chemically and physically as identical as possible, have well-characterized chemical and physical properties, and will be stable over long periods of time. Coals will be mined, transported, processed into the desired particle and sample sizes, and packaged in environments as free of oxygen as possible while maintaining the natural moisture content in order to insure that the coals will be in as pristine and stable a condition as possible.

A Users Advisory Committee is working with the Program Manager to aid in the selection of the coals to be mined, the most advantageous mining conditions, packaging for transport to the facility, methods for characterization and monitoring the stability of the samples.

The program was funded near the beginning of the 1983 fiscal year. The major amount of effort has gone into the design and construction of the coal processing facility. This part of the project is being carried out largely by personnel of the Chemical Technology Division. The process will be carried out in a facility that will be nitrogen-filled, humidity-controlled and capable of being continually purged of oxygen from the atmosphere. Stainless steel drums loaded with coal from the mines will [illegible]ed in an airlock to purge the atmosphere of oxygen before the coal [illegible] into the crusher to reduce its size to 1/4". A nitrogen cooled pulverizer will reduce the size to pass a 20-mesh screen. A siever will then screen the coal and pass it to a 45 cubic foot blender. A testing program was carried out with the blender manufacturer to establish the thoroughness of the mixing process as a function of mixing time. Tracer constituents were added to a filled and partly filled blender, and the coal was analyzed after varying times. Statistical studies were used to establish the homogeneity of the mixture.

Following a thorough mixing in the blender, the coal will be moved to a riffler for distribution to 5-gallon glass carboys for intermediate storage and to a machine to seal 20-gram samples in amber-colored glass vials. Some of the carboys will be emptied later ahead of the pulverizer, which will regrind the coal to pass a 100-mesh screen. After mixing thoroughly again, 5-gram samples of the coal will be sealed in ampoules and larger amounts in glass carboys.

A separate laboratory is being furnished to provide experimental facilities for the stability studies and related work. A large glove box will permit the handling of blocks of coal and special samples in a controlled environment for packaging and distribution to those researchers requiring these samples for their work.

2.6 Pulse Radiolysis Facility

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

   Answer: The capabilities of the Argonne electron linac (in particular, a short (< 30 picosecond) pulse duration, a high peak current (> 1000 amp), and very reliable operation) provide a powerful and unique source for the creation of unusual compounds and transient species whose properties and reactions are studied. New insight into the earliest stages of the results of energy deposition in various systems can now be obtained and studies made of the nature of and properties of excited intermediates and of the development of the subsequent chemistry. Pulse radiolysis techniques are also being utilized to measure the kinetics of gas-phase reactions of importance to combustion over a broad temperature range, to investigate the mechanism of intra- and inter-molecular electron transfer process and the action of colloidal catalysts for water splitting. The properties of the electron linac make it an ideal accelerator for investigations in other disciplines. Approximately 25% of the available beam time has been allocated for such studies as photoneutron research, testing wide bandwidth detectors for high-energy physics needs, and for the calibration of fiber optics and amplifiers. Proposals are currently being reviewed to use the facility for research and development of a free-electron laser and for installation of a positron source.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

   Answer: The uniqueness of the pulsed electron linac lies in its ability to provide pulses of short (< 30 picosecond) duration and high peak current (> 1000 amp) with a high repetition rate (1-800 pulses per second) and with high reliability. The pulse generated in this facility is approximately an order of magnitude more intense than that of any other linac in the world.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

   Answer: The Argonne Linac has detection equipment for measuring fast kinetic processes with a time resolution better than 10 ps (picosecond) for the fastest technique. The stroboscopic pulse radiolysis system and the fast streak camera system allow the measurements of chemical kinetic processes using absorption and emission with time resolutions of better than 30 ps. A spectrophotometric apparatus allows kinetic measurements over a wide time and wave-length range. The measurement of simultaneous spectra and kinetic decay enables one to quickly find important regions to study using other techniques and to make measurements using rare, expensive or radioactive compounds. Time-resolved conductometric measurements can be made for studying ionic systems.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

   Answer: Previous studies of electron transfer reactions in fluids have not shown the strong energy dependence that had been theoretically shown. By creating radicals in a rigid matrix through the use of an electron beam and thus being able to separate electron transfer reactions from diffusional processes, it was shown that electron transfer rates were maximal at about 1 eV of exothermicity as had been predicted by theory.

The rates of electron transfer reactions have been measured as a function of exothermicity and distance through the use of rigid steroid molecules with two reactant centers. An electron from the electron beam attaches to one end of the molecule and the migration of the electron to the other end of the molecule is then observed. This gives the electron transfer rate as a function of distance, and, by changing the reactant groups, the rates can also be studied as a function of exothermicity.

Future studies in electron transfer will address the corollary problem of hole (or positive ion) transfer and for effects of magnetic fields in reactions of radical pairs.

Third body effects have been found for the reaction of OH (reactive hydroxyl radicals) with CO (carbon monoxide) at high temperatures. Since these reactions are critical reactions in understanding the combustion process, and since these reactions have only been measured previously at low pressures where the reaction rates are much slower, these data are of great importance to the understanding of the chemical processes in flames.

Previous studies have only observed the disappearance of OH in the reaction of OH with CO. The intermediate HOCO is a stable radical, and little is known about its lifetime. The lifetime may be very dependent on the mechanism of its formation. The production of the final products from this reaction, in particular, the H atom, will enable us to determine the lifetime of the intermediate and from that learn about the reaction mechanism for the OH radical with CO.

Many other free radicals, which are of great importance in flame chemistry, can easily be produced through pulse radiolysis. There has been little previous work on the CH radical, and we plan to study these reactions as a function of temperature.

The fundamental processes by which energy is transformed from kinetic energy of an ionizing particle to chemical energy in liquids is being studied. One of the primary processes occurs through the ionization of a solvent molecule to form a positive ion and an electron. The distance from the positive ion at which the electron is thermalized has been measured in hydrocarbon solvents. This distance will determine the probability of reaction with other species in solution (such as proteins or nucleic acids in living systems) relative to the probability of recombination of the positive ion with the electron and no net chemical reaction.

In fluids the electron can react prior to its thermalization. The mechanism (or mechanisms) by which this reaction takes place is not understood but present studies in alcohols as a function of temperature may clarify the mechanism. Reactants such as nitromethane, benzene, and acetone in n-propanol will be studied as a function of temperature (from room temperature to -110°C).

DC conductivity can allow the probing of ionic processes in fluids which cannot be measured in other ways. These conductivity methods have allowed the clarification of mechanisms in inorganic chemistry by showing the production and loss of protons and of the energy deposition processes in hydrocarbons by studying geminate recombination kinetics.

Previously unknown oxidation states of actinide elements in aqueous solution have been prepared and identified. For example, the series Am^{+2}, Cm^{+2}, and Cf^{+2} has been studied. Absorption spectra and lifetimes for these unusual species have been obtained. During FY 1984 and FY 1985, the study of Bk^{+2} will be attempted.

We observed that radiolysis reduction of U^{+6}, Np^{+6}, and Pu^{+6} does not occur in near-neutral carbonate solutions, as would be present in deep ground waters. This is particularly important for assessment of the mobility of actinide elements following a possible break in a radioactive waste repository container.

The mechanism of the action of colloidal catalysts in H-atom reactions relevant to water-splitting has been established, and semiconductor carriers have been evaluated and utilized to optimize the efficiency of metallic colloidal catalysts. Our attention will now turn to attempts to understand the more complex, four-electron oxidation process of water to form oxygen.

5. What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?

Answer: Linac improvements have been designed and installed which increase the pulse from about 8 nanocoulombs in 25 ps to 25 nanocoulombs in 25 ps. This pulse is approximately an order of magnitude more intense than any other linac in the world. A high-speed streak camera has been purchased and is being used for beam diagnostics.

A new picosecond pulse system, using a unique compression technique, will be built. This will give us a 5 ps pulse with a current of 1000 amperes.

6. For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).

Answer:

(Budget Authority in Thousands)

	FY 81	FY 82	FY 83	FY 84	FY 85	Source of Funds
	0	0	28	28	28	High Energy Physics
	65	45	0	0	0	Nuclear Science
	505	515	532	572	612	Chemical Sciences
Facility Operation	570	560	560	600	640	
In-House Research	1570	1740	1895	1995	2040	Chemical Sciences
Out-House Research	60	55	55	60	60	Chemical Sciences
Capital Equipment	52	164	30	93	145	Chemical Sciences

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer: None

8. **For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.**

Answer: Past and projected levels are as follows:

	FY81	FY82	FY83	FY84	FY85
Man Years (Operations)	4.0	4.0	4.0	4.0	4.0
Man Years (Research)	13.2	11.8	13.3	14.2	13.7
Total	17.2	15.8	17.3	18.2	17.7

9. **What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?**

Answer: The utilization factor each year has been 75% to date and this factor is expected to remain unchanged through FY 1985 (Full utilization is determined by available funds for operation; currently this is 16 hrs. per day, 5 days per week.)

10. **For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?**

Answer:

Number of experiments started	390
Number of experiments continued	35
Number of experiments completed	355

11. **What is this facility's user policy?**

Answer: The facility, though not a formally-designated user facility, is open to all qualified users, and experiments by outside users are encouraged. Potential users arrange an experimental schedule appropriate for the user and in-house scientists. The majority of such experiments are collaborations with in-house scientists.

12. **For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?**

Answer:

Budget Authority in Thousands

	FY81	FY82	FY83	FY84	FY85
Reimbursable Research	0	0	17*	0	0

* Lawrence Livermore Laboratory

13. **What is the mechanism by which specific research proposals for experiments at the facility are considered?**

Answer: Qualified scientists are encouraged to take advantage of the specialized resources available at the Pulse Radiolysis Facility. Prospective participants should submit a brief summary of the research to the Chemistry Division Director. Criteria for selection include technical merit, overlap with DOE program objectives, and the availability of specific equipment.

14. How many research proposals have been submitted over the past five years, and how many of these have been approved?

Answer: Approximately 25 experiments have been arranged over the past five years in collaboration with outside users.

15. How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?

Answer: Twelve (12) university researchers have utilized the facility.

16. How many industrial researchers have utilized the facility over the past five years?

Answer: Three (3) industrial users have utilized the facility.

17. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer: Sixteen (16) researchers from foreign institutions have been users of this facility.

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: None. ("Researchers from other agencies" are defined as regular employees of agencies, federal or state, other than DOE or GOCO contractors.) It should be noted that scientists from other DOE laboratories use this facility.

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: There are many potential future development possibilities for the existing Pulse Radiolysis Facility, but there are currently no specific plans to undertake any of them beyond the construction activities identified in the FY 1985 budget request.

20. Please provide a copy of the facility's latest annual report.

Answer: No formal reports on facility use are prepared, since this is not operated as a formal user facility. Reports of research accomplishments, which include the work of outside collaborators and users, are prepared for DOE - Chemical Sciences in the Field Task Proposals and in an annual report, "Surveys of Research in the Chemistry Division" prepared for our Review Committees and general interest. A copy of the relevant pages from the most recent "Surveys of Research in the Chemistry Division" is enclosed.

I. **RADIATION CHEMISTRY AND PHOTOCHEMISTRY** (A. D. Trifunac, M. Beno, R. Clarke, S. Gordon, C. D. Jonah, V. Krongauz, S. Lefkowitz, D. McDonald, D. Meisel, J. R. Miller, W. Mulac, M. C. Sauer, Jr., K. H. Schmidt, P. Walsh, A. Bromberg, A. Ravon, J. C. Sullivan*, M. C Thurnauer*)
Outside Collaborators (D. M. Bartels, G. L. Closs, R. Cooper, E. Deutsch, P. Feng, E. Hart, R. G. Lawler, M. Matheson, M. Root)

The activities of the Radiation Chemistry and Photochemistry Group represent a major, dynamic effort to understand the basic chemistry and physics of processes which occur with the passage of ionizing radiation through matter. These processes are the consequence of charge separation. Charge separation together with subsequent charge transfer and recombination produce a variety of transient species, such as radicals, radical ions and excited states.

Charge separation is also the fundamental process in the conversion of light energy into chemical energy. To produce efficient energy-conversion systems, it is important to understand the basic chemical and physical processes in order to enhance energy-producing charge separation and to prevent energy-wasting charge recombination.

Experimentally, ionizing radiation is produced or induced with the Argonne electron linac, the Van de Graaff accelerator or lasers of different types. The short-lived, highly reactive species produced by the radiation are studied with state-of-the-art, time-resolved detection methods, which include both optical and magnetic resonance techniques.

For this survey, our research has been grouped under the following five topics:

A. Radiation and Photoionization.
B. Aqueous Radiation Chemistry.
C. Energy Conversion and Storage.
D. High Temperature, Gas-Phase Kinetics Related to Combustion.
E. Long Distance Electron Transfer.

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*Collaborator from another ANL-CHM group.

A. Radiation and Photoionization (A. D. Trifunac, C. D. Jonah, S. Lefkowitz, D. B. McDonald, M. C. Sauer, Jr., S. Gordon, K. Schmidt, R. Cooper)

The Argonne Radiation Chemistry program is concerned with understanding the basic processes that occur when ionizing radiation interacts with matter. Both high energy electrons and photons are utilized to accomplish the primary charge separation. The primary charge separation, charge scavenging and recombination represent the typical and dominant processes which then determine all the chemical consequences of ionization. While there is still much to be learned about the fast processes in radiation chemistry of water and other polar liquids, the non-polar liquids represent the experimentally accessible area for studies of primary charge separation. Due to weak solvation and long range electrostatic interaction between charged particles in non-polar solvents, most events occur on a very short time scale. To study these events, therefore, requires maximum time resolution in both methods of excitation and detection. The Argonne picosecond electron linac and the current development of picosecond UV lasers are the essential tools for this work. Various studies of initial events in both ionization and photoionization, the time evolution of excited states, positive ions and electrons and the kinetic consequences of the initially non-homogeneous distribution of ions are all part of our concerted effort at unraveling the chemistry and physics of energy deposition.

(1) Picosecond Pulse Radiolysis (C. D. Jonah, M. C. Sauer, Jr., S. Gordon, K. H. Schmidt)

Over the last several years, experimental and theoretical advances in energy deposition research have complemented each other. Theoretical advances which can make predictions about spur decay in water were shortly followed by experimental measurements which allowed one to test the limits of these calculations (and in many cases to find these calculations wanting). In the last few years, theoreticians have been modeling the steps in the energy deposition process. These modeling calculations include the determination of thermalization distances and the initial spatial distribution of ions and radicals, and require new or more accurate experimental results, both as input to the theory and to test the results of the calculations. Experimentally we cannot realistically expect to be able to measure all of the important processes in any given system, at the present time. For instance, in polar media where diffusion is relatively slow (tens of picoseconds) there is a large difference in time between the reactions in the spur and reactions of the precursors of the normal chemical species such as the dry electron. Thus it is relatively easy to trace the reactions of precursors in polar media compared to hydrocarbon fluids, where the normal geminate reactions are so fast that it is difficult to isolate the precursor reactions. On the other hand, the initial distribution of ions is much easier to determine in hydrocarbons since coulombic attraction dominates the recombination process and the recombination time is thus a far more sensitive function of distance than in polar media, where diffusion dominates the recombination kinetics. The very fast time resolution enables one to study unusual or unstable species which cannot be studied in other ways. These studies contribute to the entire field of chemistry. Picosecond studies are also of practical importance for the understanding of radiation effects in biological systems, or in reactor cooling systems where the description of the processes occurring at high concentrations is needed. To delineate such processes, it is important to characterize the primary species, since it is the reaction of these species that determine the early time reaction pathways which occur at high concentrations.

The unique capabilities of the Argonne linac have made possible many such experiments, since it was the first linac with a subnanosecond pulse and sufficient current to do chemistry. In the last year, a new, very fast streak camera was added to the measurement equipment on the linac. This addition, together with the present microchannel-plate photomultiplier detector, a very fast photodiode, and the stroboscopic pulse-radiolysis equipment, gives us the ability to perform fast emission measurements, measurements which are limited by the pulse width of the linac and not by the analysis equipment. The variety of detection techniques allows us to tailor the experimental system to the chemical system rather than the reverse. Following are the outlines of some of our specific endeavors.

(a) Non-Polar Liquids. The experiments in non-polar liquids have two goals: to understand what happens at early times in radiation chemistry, and to study the production and characterization of unusual chemical species.

These goals are not mutually exclusive, since many unusual species are created at very early times in radiation chemistry.

We have exploited the absorption of the hydrocarbon positive ion which we observed and characterized previously. We have studied the reactions of the positive ions of cyclohexane and n-hexane with triethylamine and found comparable rate constants (about 4×10^{10} $M^{-1}sec^{-1}$), which are larger than one would predict for species with normal mobilities. This means that there may be a high mobility species in both cyclohexane and n-hexane, a fact which had not been previously known. A cell has been developed with much thinner windows (to reduce interference from radiation-induced absorption in the windows) so that we can more accurately measure the recombination processes. We are using this cell to measure geminate processes in several different hydrocarbons.

One critical question in radiolysis concerns the number of ion-pairs created in a single ionization sequence (spur). To try to find out whether there are more than one, we have measured the yield of triplets in several hydrocarbons, including tetramethylsilane. These measurements give no evidence for more than one ion pair in a spur.

(b) Polar Liquids and Solids. While the overall radiation chemistry of polar media is reasonably well understood, there is one major uncertainty in the fundamental processes - the transition of a free electron to the solvated electron. Contrary to the common assumption that the reactivity of the electron precursor with a scavenger is similar to the reactivity of the solvated electron with the same scavenger, we find, for instance, that $LiNO_3$ and $NaNO_3$ react almost identically with the precursor of the solvated electron in ethanol, but that there is an order of magnitude difference in their reactivity with the solvated electron. This difference in reactivity is thought to arise from charge effects which are important for the solvated electron reaction but not for the precursor reactions. We have studied the solvation of anions in polar media. These data can be compared with our previous electron solvation experiments. While the solvation times for anions as a function of the solvent are strongly correlated with the solvation of the electron in the same solvent, the times are much longer than the electron solvation. This difference in solvation times means that the same processes probably occur for electrons and anions but the larger anions hinder the reorientation of the solvent.

(2) Photoionization in Dielectric Liquids (M. C. Sauer, A. D. Trifunac, D. B. McDonald, K. H. Schmidt, R. Cooper)

The photoionization of solutes such as anthracene (A) in non-polar solvents (e.g., cyclohexane or n-hexane) is being investigated as part of our general effort to understand the process of geminate-ion recombination. We have used a DC-conductivity technique to observe the conductivity changes induced by high intensity, 20-nsec duration, laser pulses at 248 nm. In a system of 2 x 10^{-6} M anthracene in cyclohexane, with 0.05 M SF_6 to rapidly capture electrons, an unexpectedly large conductivity signal, lasting about 1 µsec was observed. Effects of positive-ion scavengers, and other considerations, have established that this signal is due to the cyclohexane positive ion, which is known to have a high mobility.

In similar systems using n-hexane, which has a "normal" mobility positive ion, we do not see an anomalously large early conductivity signal. However, a signal was observed at early times. This signal was larger than expected on the basis of the observed free-ion conductivity and decayed with "geminate" kinetics. This result was unexpected because the DC-conductivity method had been thought to be completely insensitive to geminate ion-pairs. A theoretical treatment of this problem, showing that the latter concept is incorrect, is given in the following section of the survey.

Returning to the case of cyclohexane, the energy level diagram in Figure I-1 indicates why the production of the solvent ion was not expected, i.e., the absorption of two photons of 248 nm light by anthracene is expected to produce A^+, which on energetic grounds will not transfer charge to the solvent. As indicated in Figure I-1, absorption of a photon by the lowest vibrational level of the first excited singlet state of anthracene (A^1) would create an excited state of A^+ with an initial energy greater than the solvent ionization potential; hence, solvent ionization is energetically possible. However, the absorption of light by A^1 would normally be expected to result in ejection of an electron, leaving A^+ in an energy level too low to result in charge transfer to the solvent.

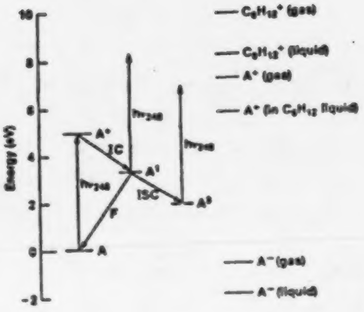


Figure I-1. Energy levels of importance in the production of ions by high intensity pulses of 248 nm light in solutions of anthracene in cyclohexane.

It appears that the light absorption by A^1 must produce the cyclohexane ion in a concerted process involving a cyclohexane molecule. According to H_2 production measurements, reaction (I-1),

$$A^1 + C_6H_{12} + h\nu_{248} \longrightarrow A^- + C_6H_{12}^+ , \qquad \text{(I-1)}$$

is favored rather than a similar reaction in which e^- is produced in place of A^-. Hydrogen production would be expected if e^- and $C_6H_{12}^+$ were produced (as is true in the case of pure cyclohexane), and our measurements show that the light absorption by anthracene leads to no increase in H_2 production.

Reaction (I-1) seems to have the disadvantage that, by its nature, the A^-, $C_6H_{12}^+$ pair would be unlikely to have an appreciable probability of separation. However, measurement of the fraction of the laser power transmitted through the sample shows that each anthracene molecule in the path of the light accounts for 10 photons absorbed. Reaction (I-1) allows this, because of the expected rapid recombination of A^- and $C_6H_{12}^+$ to produce A^1. A small probability of separation could therefore be "amplified" by a factor of 10 due to this recycling; and, in fact, the effect of light intensity on the $C_6H_{12}^+$ signal is in agreement with such a process.

Experiments with 9,10-dimethyl anthracene are planned; its excited singlet state does not cross over to the triplet state with an appreciable probability, but the energy levels (Figure I-1) are essentially unchanged. Thus, we will look for an expected enhancement of the $C_6H_{12}^+$ signal, i.e., in anthracene, the triplet state can only lead to $e^- + A^+$ according to Figure I-1.

Experiments related to the occurrence of reactions such as reaction (I-1) are planned using optical detection techniques with much better time resolution. The development of the apparatus for this is described in an accompanying section. One aim is to determine whether solvent ionization via light absorption induced by solutes is a process of general importance.

(3) Model Calculation of Geminate Ion Recombination and DC Conductivity

(K. H. Schmidt)

Microwave (MW) conductivity techniques are often used to study ion formation and decay in hydrocarbon systems. DC techniques, as described in the previous section, have also been used recently at this and other laboratories for the same purpose. DC measurements have a higher intrinsic sensitivity, are more convenient to use, and provide a higher absolute accuracy. However, a MW conductivity signal is easy to interpret since it is simply proportional to the total number of ions present at any given time, whereas the interpretation of DC conductivity is less obvious. Until this work, there was no consensus about the effect of geminate recombination on the measured DC signal, and many believed that DC techniques could not be used to study systems where geminate ion recombination predominates.

To clarify this important question, we have started a theoretical investigation of conductivity. We created a simple stochastic model that provides an understanding of the underlying mechanism, and allows one to predict or interpret the result of a DC-conductivity experiment.

The model assumes that the motion of the ions consists of three linearly superimposed components:

(1) Brownian motion,
(2) motion due to a coulombic attraction,
(3) motion under the influence of an external electric field.

In a Monte Carlo calculation carried out on the Chemistry Division's VAX 11/780 computer, each of a large number (up to 50,000) of ion pairs is assigned, initially, a random orientation, and a random distance according to a selected distribution function (delta, Gaussian, or exponential). The motion of the individual ions, as a function of time, is then traced until the end of the desired epoch, or the recombination of the ion pair. The contributions of the individual ions in the DC current (which are proportional to their velocity component in the external field direction) are also calculated and stored. Upon recombination, an ion pair is removed from the calculation. The contributions to the DC current of all ion pairs are then added, and the resulting DC conductivity calculated. Also calculated, for comparison, is the MW conductivity. In Figure I-2, the results of such a calculation are plotted. The upper curve represents the MW conductivity, the lower curve, the DC conductivity. The dashed line marks the free ion limit, calculated with the aid of the Onsager relation,

$$P(r_0) = e^{-r_0/r_c}(1 + E/E_D),$$

where r_0 is the initial distance of the ion pair; P, the probability of escape; r_c, the so-called Onsager radius, a function of temperature and dielectric constant; E_D, the "doubling field", a function of the same quantities; and E, the external electric field.

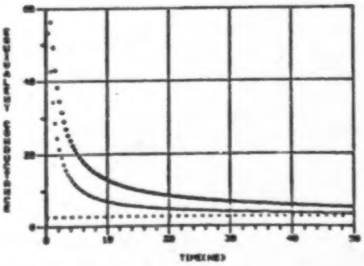


Figure I-2. Monte Carlo calculations of a DC and a microwave (MW) conductivity signal in pulse-irradiated CCl_4. Dotted curve, DC signal; diamonds, MW signal; dashed line, free-ion limit.

A stringent test for the Monte Carlo model calculation is the requirement to correctly predict the free ion yield. Figure I-3 shows that this requirement is met. The two linearized plots of MW conductivity vs. $\tau^{-0.6}$ (τ=Dt/r_c, D=diffusion coefficient), calculated for different electric fields, indeed extrapolate to the correct free ion limit.

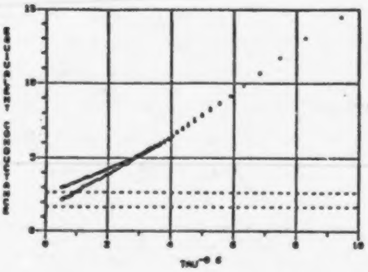


Figure I-3. Linearized plots (see text) of two calculated microwave conductivity signals. Upper curve, calculated for a DC field of 12.5 kV/cm, lower curve, calculated for zero field. The dashed lines correspond to the respective free-ion yields derived with the Onsager relation.

Figure I-4 shows a first attempt to fit actual experimental data obtained in hexane containing SF_6 as electron scavenger and anthracene. The solid and dotted lines were calculated for free ion yields of 3% and 6%, respectively (by properly choosing the average initial distance), and the circles indicate the experimental signal. The deviation at longer times is due to the fact that the model does not take into account bulk reactions of the ions.

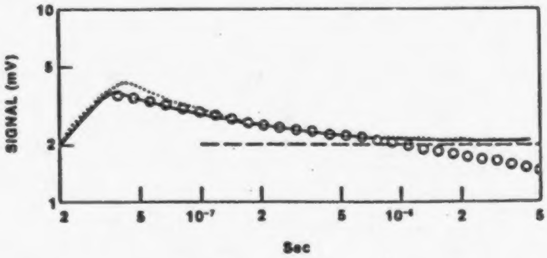


Figure I-4. Comparison between calculated DC-conductivity signals and experimental data obtained in n-hexane containing 10^{-6} M anthracene and 5 x 10^{-2} M SF_6, irradiated with a 25-ns pulse from an excimer laser. Dotted curve, 3% free-ion yield; solid curve, 6% free-ion yield; circles, experimental values; dashed line, free-ion limit.

Attempts are being made to make the calculations more efficient and to further assure their validity. We will then use the model to evaluate experiments carried out at our laboratory. Also, a cooperation has been established with the Radiation Chemistry Group at the Interuniversity Reactor Institute in

Delft, the Netherlands, and we will compare theoretical and experimental results from the two laboratories.

(4) Magnetic Resonance Studies of Radical Ions in Hydrocarbons
(A. D. Trifunac, S. Lefkowitz)

We have utilized time-resolved-fluorescence-detected magnetic resonance (FDMR), a technique developed in this laboratory, to study the structure and dynamic behavior of radical ions formed in the pulse radiolysis of non-polar solutions. FDMR yields the EPR spectra of radical ion pairs which recombine to form a fluorescent neutral species. This technique combines the advantages of fast time resolution (ca. 50 nsec) and unique sensitivity to radical ions, allowing the measurement of the EPR spectra of these transient species without interference from other paramagnetic species present.

Our particular interest has centered around solutions in cyclohexane, a solvent which has long been considered a prototypical alkane in radiolysis, but has recently been found to possess a radical cation (hole) species with an anomalously high mobility (ca. 50 times faster than diffusion controlled). Little is known concerning the nature of this high mobility hole, or of other hole species that might be present in irradiated cyclohexane solutions.

In Figure I-5 we show the FDMR spectrum of a solution of the scintillator 2,5-diphenyloxazole (PPO) in cyclohexane, measured within 200 nsec of the ionizing radiation pulse. The spectrum shows a narrow center peak along with broad, structured shoulders. Examination of the shoulder spectrum suggests that it belongs to the EPR spectrum of the cyclohexane radical cation, and consists of a double-septet pattern (stick spectrum) arising from the hyperfine interaction of the six axial and equatorial protons with the unpaired electron. This result was confirmed by comparison with the conventional EPR spectrum of cyclohexane in freon, irradiated and measured at 77 K; and provided the first EPR evidence for the participation of alkane radical cations in the radiation-induced fluorescence of scintillator solutions.

A more striking inference which may be drawn from the appearance of well-resolved features in the cyclohexane hole FDMR spectrum is that this species is definitely not the mobile species identified previously by conductivity methods. Hence, we have observed, for the first time, a physically trapped

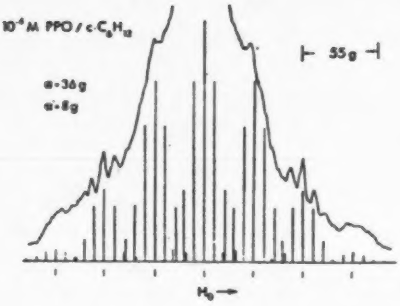


Figure I-5. Fluorescence-detected magnetic resonance (ESR) spectrum of radical ions $PPO^{-\cdot}$ and c-$C_6H_{12}^{+\cdot}$ in the solution of 10^{-4} M PPO in cyclohexane. The stick ESR spectrum illustrates the assignments of c-$C_6H_{12}^{+\cdot}$ ESR transitions with the hyperfine coupling constants indicated.

cyclohexane radical ion, with a "normal" mobility, that has not undergone any chemical reaction or rearrangement.

We have further investigated the properties of cyclohexane holes using triethylamine (TEA), which is believed to scavenge the alkane hole according to the reaction,

$$\text{TEA} + \text{Alkane}^{+\cdot} \longrightarrow \text{TEA}^{+\cdot} + \text{Alkane}, \qquad \text{(I-2)}$$

with the resulting triethylamminium radical recombining with the scin-tillator radical anion to yield fluorescence. Figure I-6 shows the FDMR spectrum of an irradiated solution of PPO and TEA in n-hexane. The well-resolved shoulder peaks were assigned to the previously unreported $TEA^{+\cdot}$ EPR spectrum, and are composed of overlapping hyperfine splittings of the nitrogen triplet with the six equivalent β protons. Tripropyl and tributylamines also give similar FDMR patterns with slightly different splittings, providing additional proof for our EPR assignments.

We exploited the time resolution of FDMR to resolve kinetically the scavenging of the cyclohexane hole species by TEA. We did this by measuring the intensity growth of the $TEA^{+\cdot}$ peaks at increasing times following pulse irradiation. The rate of intensity growth was quite similar to that in cyclohexane and n-hexane in which the hole mobility is diffusion controlled. This intriguing result indicated that TEA only scavenges the trapped cyclohexane

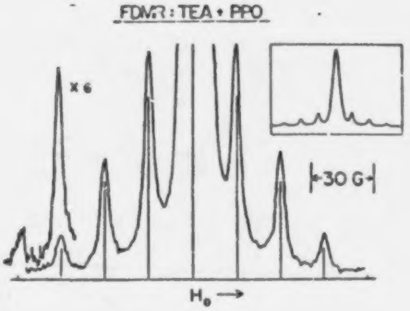


Figure I-6. Fluorescence-detected magnetic resonance (ESR) spectrum of radical ions $PPO^{\bar{\cdot}}$ and $TEA^{\dot{+}}$ in the solution of 2 mM TEA and 1 mM PPO in n-hexane. The stick ESR spectrum illustrates the assignments of TEA^{+} ESR transitions.

hole species to form $TEA^{\dot{+}}$, and that its reaction with the mobile hole, measured by conductivity, does not detectably yield $TEA^{\dot{+}}$.

In summary, we have used FDMR to identify the participation of alkane radical cations as precursors to scintillator fluorescence in pulse radiolysis. We have derived both structural and kinetic EPR evidence for the presence of a physically trapped cyclohexane radical cation, a species whose existence must be considered in any future theories of hole transport in cyclohexane. In the course of these studies, we have also obtained the first EPR spectra of several trialkylamminium radicals. Most generally, substantial progress has been made in demonstrating the utility of FDMR in studying primary processes in the pulse radiolysis of non-polar scintillator solutions.

(5) Picosecond Photolysis - Photoionization (C. D. Jonah, D. B. McDonald)

As a complementary part of our effort to characterize the transient species produced in radiolysis and to understand their early time behavior, we are developing a program of picosecond pulse photolysis. The experimental system pivots on the ability of mode-locked lasers to generate time-bandwidth limited pulses of 0.03 to 100 ps in duration. Although the present goal of 5-20 ps is easily reached at tunable wavelengths as short as 285 nm, such wavelengths are not extremely useful in photolysis or photoionization in any but a special class of molecules. The main thrust in the development of our experimental system is the generation of tunable ionizing radiation in the wavelength range from 100 nm to 285 nm. We have incorporated a copper-vapor laser pumped amplifier into a synchronously pumped dye-laser system in order to achieve the high peak intensities necessary for the nonlinear optical generation of intense hard UV pulses (see Figure I-7). A high repetition rate system has been chosen to facilitate signal averaging and alternate detection techniques such as time-correlated photon counting.

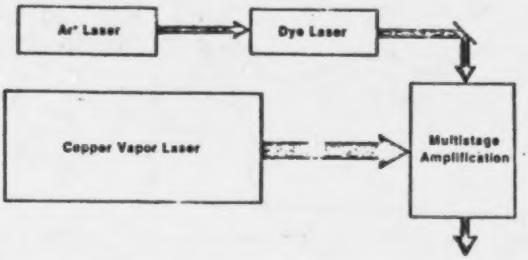


Figure I-7. Schematic for picosecond vacuum UV pulse generation. The mode-locked argon-ion laser synchronously pumps a dye laser which provides pulses from 5-ps to 20-ps duration. The 5-KHz copper-vapor laser amplifies the pulses to power levels suitable for nonlinear optical techniques. Our design features a high repetition rate and flexible means of producing synchronized probe light at various wavelengths. Pulses with greater than 5 MW peak power have been achieved.

One of the first systems to be studied will be the 2-photon ionization of anthracene solutions in cyclohexane. Transient conductivity measurements after irradiation with 20-ns excimer laser pulses at 240 nm have indicated that the solvent can be ionized with a second photon when the first is absorbed by the solute. The identification of the solvent ions by conductivity is peculiar to cyclohexane. Spectroscopic identification of transient products will allow similar studies in other solvents; tunability will allow other solutes; and the time resolution will help elucidate the mechanism of this unusual cooperative event.

The experimental system is designed to be versatile enough to study many other photochemical systems in all phases.

B. Aqueous Radiation Chemistry (A. D. Trifunac, D. M. Bartels, S. Gordon, W. A. Mulac, M. C. Sauer, Jr., K. H. Schmidt, L. R. Morss*, J. C. Sullivan*, D. Wester*, P. Feng, E. J. Hart, R. G. Lawler)

A study of the aqueous radiation chemistry of radicals, atoms and metals is a clean and direct way of obtaining the details of reaction mechanisms. The topics listed below illustrate many diverse aspects of radiation chemistry studies. The study of the aqueous radiation chemistry of the actinides by pulse radiolysis is an excellent example of how chemistry relevant to separations and storage is being developed. The study of oxygen ($O(^3P)$) production utilizes both radiation chemistry tools and lasers to address the reaction mechanism, which is of importance in water radiolysis. The time resolved EPR study of aqueous solutions uses spin to assess collision dynamics of reactive radicals in liquids. This effort is closely tied to a continuing evolution of our specialized magnetic resonance tools.

(1) Actinides (S. Gordon, W. A. Mulac, K. H. Schmidt, L. R. Morss*, J. C. Sullivan*, D. Wester*)

This work is part of an ongoing program in which we study the physicochemical properties of actinides and lanthanides in aqueous solution. In particular, we study the various stable and unstable valence states of the ions and the structural transformations in going from one valence state to another, hydrolytic properties of the ions (pK values), redox potentials, and kinetic data. The main goal is to understand the reactions of these elements in the aquatic environment and in a number of areas of process chemistry. The program is carried out in collaboration with the Heavy Element Chemistry Group, using our unique pulse-radiolysis facilities at the Chemistry Division electron linac.

(a) Reduction of Cf(III) to Cf(II) by the Hydrated Electron. We have succeeded in producing Cf(II) by the pulse radiolysis of an aqueous solution of Cf(III) by reaction with the hydrated electron. Californium was present as the perchlorate at a pH of ~5.2. Figure I-8 shows a time-resolved spectrum of Cf(II). The spectrum shows a broad absorption increasing from 440 to 260 nm. The rate constant of formation of Cf(II) is greater than 3 x 10^{-9} $M^{-1}s^{-1}$. The Cf(II) disappears with an apparent first-order rate constant

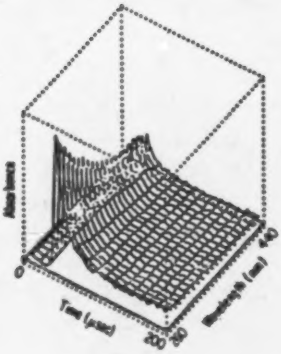


Figure I-8. Time-resolved optical absorption signal obtained hy pulse-irradiation of a He-saturated solution of 0.0005 M $Cf(ClO_4)_3$ at pH 5.3 containing 0.1 M t-butanol.

of 7×10^4 sec^{-1}. We should note that this value is similar to that previously determined for the oxidation of Am(II) (9.7×10^4 sec^{-1}) despite the $5f^7$ configuration of the latter as compared to $5f^{10}$ for Cf(II).

(b) Reaction of Actinides in Carbonate Solution. We have applied the Marcus cross relations for outer sphere electron transfer reactions to calculate the rate constants of the reactions,

$$CO_3^{\cdot -} + An(V)\cdot 3CO_3^{=} \longrightarrow CO_3^{=} + An(VI)\cdot 3CO_3^{=} \quad , \qquad (I\text{-}3)$$

where An stands for U, Np, or Pu.

The calculations were made using the redox potentials for these elements obtained by cyclic voltametry. The calculated values for the rate constants of the above reactions, and those experimentally determined by pulse radiolysis, are listed in Table I-1.

Table I-1.

An	log k (calc)	log k (obs)
U	9.75	8.69
Np	7.05	7.18
Pu	7.10	7.44

For the calculation of log k we used $k_2 = 100\ M^{-1}s^{-1}$ for the self-exchange reaction,

$$^{*}CO_3^{\dot{-}} + CO_3^{2-} \longrightarrow {}^{*}CO_3^{2-} + \dot{C}O_3^{\dot{-}} \ . \qquad (I\text{-}4)$$

This value of k_2 is a recent theoretical estimate by D. Stanbury. However, a variation of k_2 within 4 orders of magnitude has a relatively small effect on the log k values.

(2) Cyclic Conjugated Radicals (S. Gordon, K. H. Schmidt, P. Feng)

(a) Cyclooctatetraene. It is known that aromatic cyclic hydrocarbons are more resistant to radiation decomposition than non-aromatic hydrocarbons. Aromatic compounds follow the Hückel rule, i.e., they have 4n + 2 π-electrons. Cyclooctatetraene (COT), with 8 π-electrons, does not fulfill this rule. Yet, liquid COT exhibits an even greater stability to radiation than benzene.

We are investigating the reactions of COT in aqueous solution with the OH radical, the H-atom, and the hydrated electron to create radicals with various numbers of π-electrons, and to study the relation between stability and structure.

In addition to kinetic data and spectra for the radical anion of COT and H and OH adducts, we now have evidence for the formation of the dianion in a second order reaction of COT^-, presumably by disproportionation:

$$2COT^- \rightleftharpoons COT^{=} + COT \ . \qquad (I\text{-}5)$$

The optically determined rate constant for this reaction is $5.5 \times 10^8\ M^{-1}s^{-1}$. Figure I-9 is a time-resolved absorption spectrum determined by our streak camera. It shows the decay of the COT^- radical anion. Note the buildup of an absorption in the minimum of the original spectrum (dashed line). Figure I-10 shows the spectrum of the same solution measured approximately 1 minute after the pulse. This spectrum has a striking similarity to the spectra attributed to the dianion produced by Na or electrolytic reduction in non-aqueous solvents.

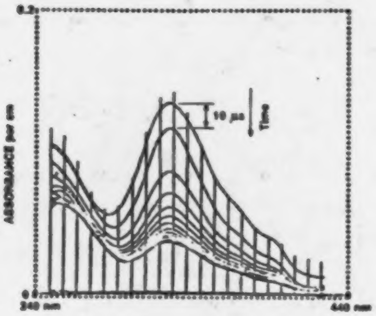


Figure I-9. Time-resolved absorption spectrum obtained in pulse-irradiated aqueous solution of cyclooctatetraene, saturated with N_2O.

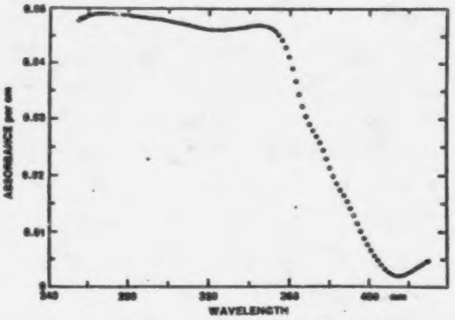


Figure I-10. Differential absorption spectrum measured ca. 1 min. after linac pulse; solution as in Figure I-9.

Figure I-11 shows a transient conductivity signal obtained at pH 10.8. The buildup of the negative part of the signal reflects the formation of COT^-. The decay of the negative conductivity signal is 3 to 6 times slower than the optically observed decay of COT^-. Since reaction (I-5) produces practically no conductivity change, this decay must, therefore, reflect the decay of the dianion produced in reaction (I-5).

We believe that $COT^=$ decays in water by reaction (I-6),

$$COT^= + H_2O \rightleftharpoons COTH^- + OH^- . \qquad (I\text{-}6)$$

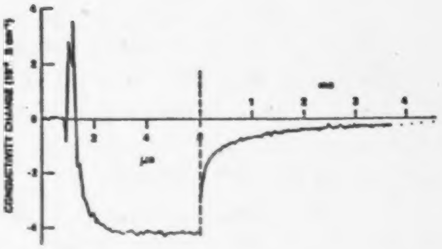


Figure I-11. Transient conductivity signal measured in a pulse-irradiated aqueous solution of cyclooctatetraene, saturated with N_2O. pH adjusted to 10.8 with NaOH.

From the amplitude of the residual conductivity signal as a function of pH, we estimate the pK_a of reaction (I-6) to be about 10.5. In the pH range studied, we did not observe a further protonation of $COTH^-$ to $COTH_2$ (cyclooctatriene). Therefore, we assume that the pK_a of reaction (I-7) is >12.

$$COTH^- + H_2O \rightleftharpoons COTH_2 + OH^- \qquad (I\text{-}7)$$

These observations are to be expected from the Hückel rule of aromaticity for the following redox system:

$$\underset{(4n)}{COT_{(tub)}} \underset{-e}{\overset{+e}{\rightleftharpoons}} \underset{(4n + 1)}{COT^{\overset{-}{\cdot}}_{(nearly\ planar)}} \underset{-e}{\overset{+e}{\rightleftharpoons}} \underset{(4n + 2)}{COT^{2-}_{(planar)}} . \qquad (I\text{-}8)$$

(b) Benzothiophene. In collaboration with P. Feng of Marquette University, we are continuing our investigation on the radiation chemistry of certain coal model compounds such as thiophene and benzothiophene. The reactions of such compounds with radiolytically produced radicals is interesting in the context of the problem of sulfur removal from coal.

Recently, we have reported the spontaneous (not acid-catalyzed) formation of a radical cation as a product of the reaction of OH with benzothiophene (BT):

$$BT + OH \xrightarrow{a} BTOH\cdot \xrightarrow{b} BT^{+\cdot} + OH^- . \qquad (I\text{-}9)$$

We also measured the rate of the reaction

$$BT^{+\cdot} + OH^- \longrightarrow BTOH^{\cdot} . \qquad (I\text{-}10)$$

We are now attempting to gain better understanding of the mechanism involved, and of the structures of the various radical species. Holcman and Sehested have determined in 1979 that log k_{1b} and log k_2, for the analogous reactions with 14 different substituted benzenes, closely follow a linear relationship with the ionization potentials of the parent compounds in question. In all these compounds, the OH radical attaches to the benzene ring.

We found that our value of k_2 for BT perfectly fits into the series of substituted benzenes, whereas our value of k_{1b} is at least 2-1/2 orders of magnitude larger than that calculated from the ionization potential of BT. This difference in k_{1b} values seems to indicate that, in our case, the point of attack of the OH radical could be the thiophene ring, followed by an internal rearrangement of the $BT^{+\cdot}$, i.e. BTOH· and BTOH·' are not identical.

(3) $O(^3P)$ in Aqueous Systems (M. C. Sauer, Jr., E. J. Hart)

The mechanism of production of $O(^3P)$, the ground state of the oxygen atom, in radiolysis and photolysis has been a subject of research in this laboratory for several years. A very sensitive method for measuring the yield of $O(^3P)$ has previously been developed; namely, the measurement of C_2H_4 produced when $O(^3P)$ reacts with cyclopentene. This method has allowed precise measurements of G-values and quantum yields.

We have recently completed an investigation of the quantum yield for the production of $O(^3P)$ from the 248 nm photolysis of H_2O_2 and HO_2^- from a pH of 3, where H_2O_2 predominates, to a pH of 13, where HO_2^- predominates, i.e., $H_2O_2 \rightleftarrows H^+ + HO_2^-$, pK = 11.6 . Light absorbed by H_2O_2 produces $O(^3P)$ rather inefficiently, the yield per quantum of light absorbed by H_2O_2 being about 3×10^{-4}; while light absorbed by HO_2^- is much more efficient, resulting in 0.08 ± 0.015 $O(^3P)$ per photon, independent of pH. The quantum yields in the case of HO_2^- were obtained by measuring the yield of $O(^3P)$ as a function of cyclopentene concentration (at each pH studied), and an extrapolation to "infinite" cyclopentene concentration by means of a linearized competition plot.

(4) Collision Dynamics of Radicals in Aqueous Radiolysis (A. D. Trifunac, D. M. Bartels, R. G. Lawler)

In recent years the time resolution of EPR spectroscopy has been advanced to its theoretical limits by direct microwave detection and electron spin echo techniques. These advances have made possible the study of EPR signals from very reactive free radicals in solution on a sub-microsecond time scale. Of particular interest in these systems are non-reactive encounters which result in spin dephasing (line broadening) and Chemically Induced Dynamic Electron Polarization (CIDEP). Observation of these phenomena constitutes a probe of the diffusive nature of the radical encounters. The characterization of collisions between reactive free radicals in solution has advanced significantly in the past year in this collaborative effort between ANL and Brown University. Radicals are produced with electron pulses from the Argonne Van de Graaff accelerator and detected in a fast response, pulsed EPR spectrometer. Electron spin echos are generated as a function of time after a radiolysis pulse to follow the radical reaction. Very large radical concentrations ($\sim 10^{-3}$ M) may be generated with this equipment, so that the echo amplitude is strongly affected by CIDEP and collisional dephasing.

Radiolysis of N_2O saturated aqueous acetate solution yields a clean, single radical system which decays by pure second order radical-radical combination kinetics. Earlier work at ANL examined the kinetic behavior of the high- and low-field hyperfine lines of the radical $\cdot CH_2COO^-$ following pulse radiolysis of 0.5 M aqueous KOAc solutions. The time-resolved signal from these lines is dominated by the polarizing effects of radical pair CIDEP. Detailed analysis of the data indicated an additional concentration-dependent mechanism which could result from the Heisenberg exchange interaction in non-reactive radical encounters.

The central acetate radical line could not be quantitatively examined earlier because of interference from a strong sample-tube background signal (see Figure I-12a). A major accomplishment of the past year has been the development of a new technique to eliminate the sample tube altogether. By introducing the sample as a free-flowing liquid jet (see Figure I-13), we have been able to observe the central line free from the effects of CIDEP (see Figure I-12b).

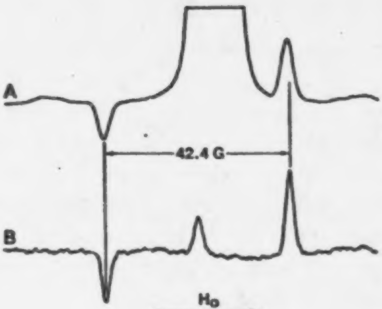


Figure I-12. Spectra of CH_2COO^- taken (A) using a standard flat EPR sample tube and (B) using a free-flowing liquid jet. Both spin-echo EPR spectra were taken of the same 0.5 M aqueous potassium acetate solution one microsecond after irradiation with a 100-ns pulse of 3-MeV electrons. In (A) the acetate radical signal (illustrating the peculiar emission/absorption effects of radical pair CIDEP) is superimposed on the broad sample tube background which completely obscures the center radical line. In (B) all three lines are easily observed.

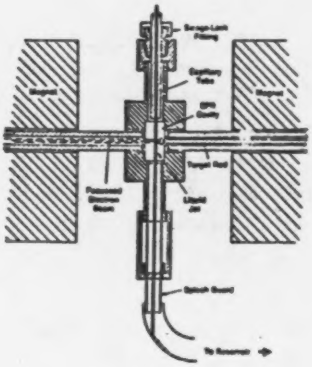

Swagelok Fitting
Capillary Tube
Magnet
Magnet
EPR Cavity
Target Rod
Focussed Electron Beam
Liquid Jet
Splash Guard
To Reservoir

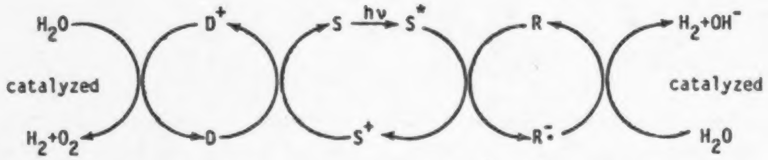
Figure I-13. Diagram of the EPR cavity modified to admit the electron beam and free-flowing jet. Sample liquid is pumped vertically downward through the microwave cavity and caught in a plastic tube mounted below. Gravity flow returns the solution to a sample reservoir below the spectrometer. The electron beam enters the apparatus horizontally along the center axis of the magnet and crosses the jet in the center of the cavity. Elimination of a sample tube by this technique makes possible much higher electron-pulse repetition rates and faster data collection since the jet remains stable under high dose conditions which would break a sample tube.

The additional data provided by the center line kinetics has allowed us to estimate chemical concentrations and magnetic relaxation rates with greater certainty. In addition, the jet technique allows us to use much larger electron beam currents without fear of breaking a sample tube. By pushing the radical concentration to about 10^{-3} M, we are able for the first time to detect directly the presence of non-reactive dephasing collision in a system which is reacting with a "diffusion controlled" rate.

The ratio of dephasing and reaction rates constitutes a unique measure of the reaction probability per collision.

C. Energy Conversion and Storage (D. Meisel, M. C. Thurnauer, J. C. Sullivan*, A. Bromberg, E. Deutsch, M. S. Matheson, A. Ravon, M. Root)

The design of a system which will convert and store energy in useful fuels or chemicals is based on the following scheme:



where S = light absorbing sensitizer,
R = electron acceptor relay,
D = electron donor relay.

This scheme accomplishes the desired goal of photochemical water splitting summarized by the following net reaction:

$$2H_2O \xrightarrow{h\nu} 2H_2 + O_2 .$$

The chemistry of each of the steps in the above scheme is analyzed in detail, and the various mechanisms operating in each of the cycles are studied. Once the factors controlling the chemistry of these steps are understood, effort is made to improve the performance of each component operating in tandem with the rest of the system. A battery of experimental techniques are utilized in the study of these complex and interactive chemical systems. The unique linac facility of the ANL Chemistry Division coupled with a variety of laser flash-photolysis instruments and a wide range of detection techniques provide the means to explore the systems of interest in great detail. In addition to these techniques, a variety of others are utilized when applicable to a specific step in the above scheme. These other methods include conventional kinetic techniques (e.g., stopped flow), electrochemical techniques, colloid chemistry techniques (e.g., electron microscopy), surface chemistry and others. The specific studies undertaken in this project are outlined below.

(1) Radical Pair Dynamics And Interactions In Organized Assemblies

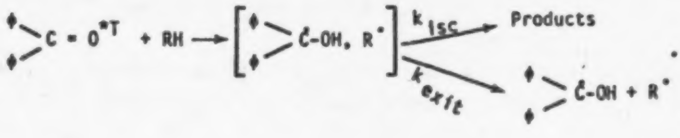
(D. Meisel, M. C. Thurnauer, A. Bromberg)

The most difficult problem in any light harvesting system is the problem of the back reaction (I-12):

$$S^{*} + R \longrightarrow S^{+\cdot} + R^{-\cdot} \qquad \text{(I-11)}$$

$$S^{+\cdot} + R^{-\cdot} \longrightarrow S + R \;\; .. \qquad \text{(I-12)}$$

Control over the microenvironment in which reactions (I-11) and (I-12) take place and some micro-organization in the system may provide the means to overcome this problem. We therefore study in detail the dynamics and the interactions of the radicals produced in reaction (I-11) in a variety of microenvironments (micelles, polyelectrolytes, vesicles, etc.). In addition to spectrophotometric and fluorescence detection techniques, we have recently employed the time-resolved, electron-spin-echo technique to study radicals and radical pairs in micelles. The reactions (I-13) of benzophenone excited to its triplet state with hydrogen donors (RH, e.g. cyclohexadiene) has been studied in SDS micelles using the latter technique:



. (I-13)

In addition to the determination of the lifetime of the radical pair (the bracketed species above) and the rates of each of its decay pathways, we were able to determine the average distance between the pair components in the pair. We have also suggested that the excitation of the ketyl radicals may result in intersystem crossing to a quartet state (Figure I-14). We now extend these studies to reactions of other ketones, e.g. quinones and benzylic ketones. In related studies, rates of electron transfer between radicals in micellar systems are being measured using the linac facility. Redox potentials of these short-lived radicals are being measured and the effects of the micelle or environment on the redox properties are being systematically investigated.

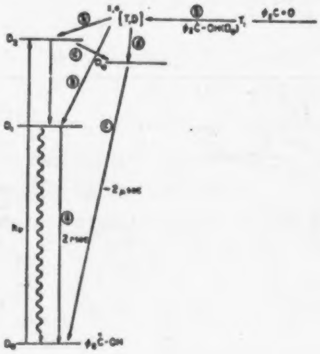


Figure I-14. Proposed energy-level diagram and excited-state lifetimes of the diphenylketyl radical.

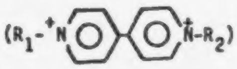
(2) Redox Catalysis In Colloidal Systems (D. Meisel, M. S. Matheson, A. Ravon)

Mechanisms of redox catalysis, primarily catalysis of water-splitting reactions, are studied in detail. Catalysts are colloidal metals, semiconductors, and their mixtures, stabilized by polymeric materials. Radicals, which provide the reducing equivalents, are produced pulse-radiolytically and their decay kinetics with the colloid are studied spectrophotometrically. The reactions of the water components (H^+ for the hydrogen evolution reaction and OH^- for the oxygen evolution) with the colloidal particles are studied by conductivity. Methods for producing colloidal catalysts by _in situ_ radiolysis and for in situ polymerization of the stabilizer are developed and their performance in photolytic systems is evaluated.

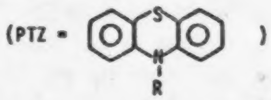
During the last year the role of the stabilizer in colloidal Pt and TiO_2 catalysts has been investigated. At very low [stabilizer]/[colloid] ratio the stabilizer induces aggregation of the particles. At too high stabilizer concentrations, the stabilizer blocks active sites on the particles. The site of adsorption of a variety of polymeric stabilizers on Ag colloids has been studied using the surface-enhanced Raman technique. Initiation of chain reactions of monomeric acrylamide derivatives by radiolysis and their propagation to form colloid-stabilized polymers are studied. The interaction of the propagating radicals with Pt in oxidation states IV-0 is presently under detailed investigation.

(3) Quencher-Ligand Interactions In Inorganic Complexes (D. Meisel, J. C. Sullivan, E. Deutsch, M. Root)

The degree of interaction of a quencher of excited states with a fluorescent inorganic complex can be controlled by the distance between the fluorescent center and the bound quencher and by the mode of binding. A study of these effects has been initiated during the last year. Oxidative quenchers of the viologen series



have been synthesized and were bound to a polymeric backbone at various distances from bound $Ru(bpy)_3^{2+}$ centers (bpy = 2,2'-bipyridine). Fluorescence yields, rates of electron transfer to the quencher and rates of back reactions have been measured. The use of such polymers in energy conversion systems and their additional role as catalyst stabilizers are evaluated. Reductive quenchers of the phenothiazine series



have been directly bound through the sulfur atom to the Ru core in complexes of the general formula Ru(bpy) (terpy) PTZ^{2+} (Figure I-15a). In such cases of strong metal-ligand interaction, the ligand loses its independent redox properties (Figure I-15b). Thus the complex is fluorescent regardless of whether the PTZ moiety is bound to the metal core. The free ligand, however, is a potent reductive quencher of the complex. The photochemistry of such complexes, rates of ligand loss, and rates of internal as well as external electron transfer are studied.

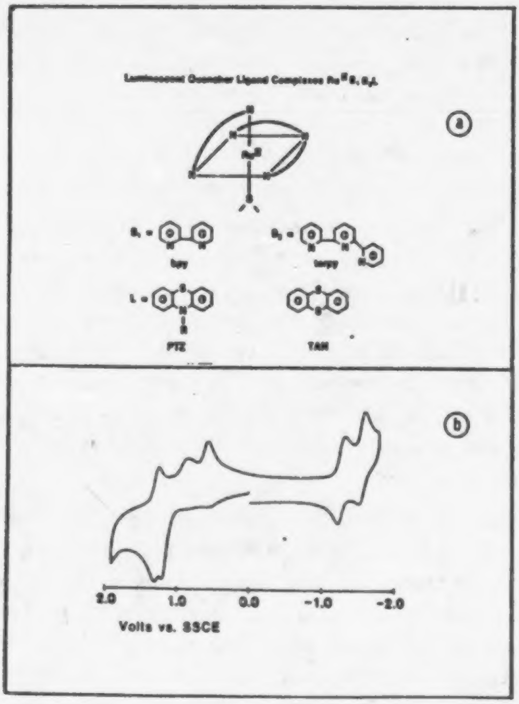


Figure I-15. (a) Structure of (terpy)(bpy)Ru^{II}L^{2+} complexes, where the free L are luminescence quenchers of the Menothiazine series. (b) Cyclic voltammogram of (terpy)(bpy)Ru^{II} (PTZ)$^{2+}$. Note two waves in the anodic oxidation region and an additional wave in the reversed scan indicating release of PTZ upon oxidation of the complex.

D. High Temperature Gas-Phase Kinetics Related to Combustion (C. D. Jonah, M. F. Beno, W. A. Mulac)

Gas-phase kinetics is important for many fields of research; for instance, free radical reactions are of importance in atmospheric and combustion chemistry, and the kinetics in gas-phase water radiolysis can help verify radiation physics models. A beam of high energy electrons can create radicals and ions cleanly and efficiently in the gas phase, and facilitates research in those fields. At Argonne we have several electron sources which can be used. The Argonne linac provides a strongly penetrating beam of electrons with a high repetition rate. This accelerator is ideal for use in high-temperature studies since the electron beam can penetrate the oven. Two Febetrons, with pulse widths of 3 ns and 40 ns, provide even higher radical concentrations and can be used for room temperature single-shot studies.

Most of the important combustion reactions are radical processes. Radicals such as OH, CH, CH_2, and NH are often difficult to make, but can be made very cleanly using an electron beam in a pulse radiolysis experiment. There is a dearth of reaction-rate measurements at room temperature, and these measurements vary sometimes by nearly two orders of magnitude. There are even fewer rate constant measurements over the wide range of temperatures that occur in combustion. We have developed a system which enables us to measure the rate constants from just above room temperature to 1300K; the upper limit is set by the melting point of quartz.

We are presently studying OH reactions which are important in the combustion process. While OH reactions have been thoroughly studied at lower temperatures and while there is a great deal of information available for testing and verifying our experimental system, there is still a great deal to learn since there have been no direct measurements above 1000K. The rate constants in the literature above 1000K have been derived from measurements in shock tubes or in flames. It is important therefore to test these reaction-rate measurements at high temperatures. We have measured OH + CH_4, OH + CO and OD + CO. In Figure I-16 we show the results (X) for OH + CH_4 and compare these data with previous experimental results. Our data are between the two most recent measurements, providing an excellent confirmation of our technique. In Figure I-17 our rate constants (X) for the reaction of OH with CO are compared with previous experimental data. There is excellent agreement between our

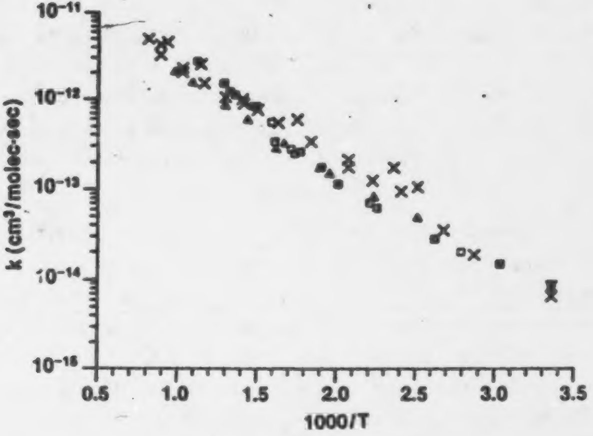


Figure I-16. Rate constant for OH + Methane. X are Argonne data. △ from Tully and Ravishankara and ⊡ from Zellner and Steinert.

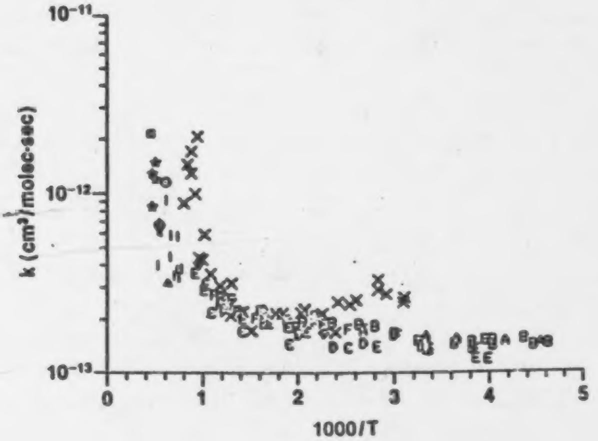


Figure I-17. Rate constant for OH + CO. X are Argonne data. ★, ⊡, |, ⊙, △, ▽ are derived measurements from shock-tube or flame measurements.

data and previous data in the range of 500-1000K, the range over which the previous data have been determined directly. Above 1000K, our data represent the only directly measured rates, and there is clearly a substantial variance between our data and the previously derived shock-tube and flame measurements. Since our data are direct and since the technique has been verified for OH + CH_4, it would appear that previous measurements of OH + CO are incorrect.

Members of the Chemistry Division Theoretical group are studying the OH + CO reaction. Tunneling of the H atom in the transition state is thought to be an important process, and the importance of tunneling can be tested by measuring the reaction rates of OD + CO as well as OH + CO. We have measured both reactions and find that the isotope effect peaks at about 500K. These measurements can clarify the microscopic reaction mechanism and do provide input to the modelling calculations in progress.

The rates and activation energies for the reactions of OH and OD with hydrocarbons and the isotope effect on both the rates and the activation energy are being determined. We plan to expand these studies to other radicals in the near future. Studies at Argonne have shown that the CH radical can be studied using pulse radiolysis, and we plan to determine rates and activation energies for CH with CO and other reactants of interest to combustion modellers.

F. Long-Distance Electron Transfer (J. R. Miller, V. Krongauz, G. L. Closs, S. Helms, K. Matusak, M. O'Neil)

This program of research has shown not only that electron transfer (ET) reactions can occur between molecules held at fixed distances (10-40 Å), but also that these fixed-distance ET reactions may be directed and controlled in ways not possible for diffusive ET reactions occurring in fluids. This direction and control is crucial to efficient energy storage in photosynthesis. The program seeks answers to fundamental questions of how distance, energy and molecular structure regulate ET rates in order to provide a basis for the design of molecular systems for efficient charge separation in photochemical solar energy storage. By providing experimental answers to these fundamental questions, this work is an important complement to the many solar photochemistry programs which explore complex systems such as micelles, vesicles, derivatized semiconductors, colloids and molecular assemblies. Measurements on those complex systems do not, in general, allow clear understanding of the basic electron transfer steps essential to their function and efficiency. We are using three experimental techniques to study rates of ET between molecules held at fixed distances. Two of these techniques rely on Argonne's picosecond linac, which is a powerful tool for studying ET mechanisms.

(1) Pulse Radiolysis Measurements of ET in Linked Molecules (J. R. Miller, G. L. Closs)

Molecules such as IV shown in Figure I-18 hold two electron-acceptor groups at a rigidly fixed distance of 16 Å center to center. The 10 Å between the nearest edges of the two acceptors is occupied by a rigid molecular spacer. When an excess electron is added to the biphenyl group of IV in MTHF (2-methyl-tetrahydrofuran) solution at room temperature, the electron transfer to the quinone group occurs in $t_{1/2} = 7$ ns. This rapid ET rate is remarkable because it is at least ten times slower than the more moderately exothermic ($\Delta G^{\circ} = -1.1$ eV) ET reaction in compound I (not shown) in which the acceptor group is cinnamoyl rather than benzoquinoyl. Rates in four compounds synthesized with biphenyl and different acceptor groups at opposite ends of steroids are shown in Table I-2.

Highly exothermic ET is slower in IV than more moderately exothermic ET in I (Table I-2). This inversion is predicted by theory but has not been found to occur in the overwhelming number of cases studied in fluid solutions. A regular decrease of rate with increasing exothermicity was observed for intermolecular ET between molecules held at fixed distances in rigid glasses. For diffusional ET in liquids, the true relationship of rates to thermodynamics becomes buried under the diffusion-controlled limit and the formation of complexes. Thus, this work provides some insight into the function of the photosynthetic reaction center, a fixed-distance array of molecules which appears to prevent highly exothermic back electron transfer by using the kind of Franck-Condon prohibitions against highly exothermic ET reactions observed here.

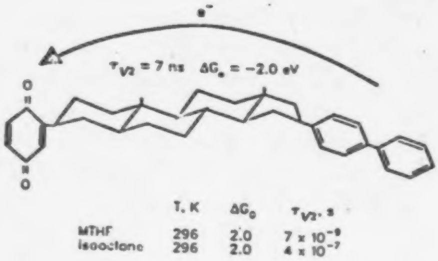


Figure I-18. Fast electron transfer occurs in difunctional molecules. This one (molecule IV) contains a biphenyl group on the right and a benzoquinone group on the left, which is more easily reduced by 2.0 eV. Addition of an e⁻ to the quinone using a 30-ps linac pulse produces a quinone radical anion, which lives for many microseconds. But there is an equal chance for the extra e⁻ to add to biphenyl, which then rapidly transfers to the quinone. In molecule IV, this transfer was measured to occur in 7 ns.

Table I-2. Electron Transfer in Rigid Bifunctional Steroids

	Acceptor Group	$-\Delta G^\circ$,eV[a]	r(Å)[b]	$t_{1/2}$(s)[c]
I	cinnamoyl	1.1	9	$<5\times10^{-10}$
II	vinylnaphthyl	0.32	9	2.5×10^{-8}
III	naphthyl	0.05[d]	10	1×10^{-6}
IV	benzoquinoyl	2.0	10	7×10^{-9}

a. Free energy change for electron transfer from the biphenyl group to the acceptor group, given by the differences in reduction potentials.

b. Separation of the nearest edges of the biphenyl and acceptor group.

c. Half-life for intramolecular electron transfer in MTHF at 296K, corrected for relatively small amounts of intermolecular electron transfer.

d. The free-energy change for the biphenyl to naphthyl transfer was obtained from the observable equilibrium in compound III. It coincides with literature values for biphenyl and naphthalene.

(2) Electron Transfer in Rigid Glasses (J. R. Miller, V. Krongauz)

The molecules ADOB and EOB shown in Figure I-19 demonstrate how solvent polarity effects can dramatically influence ET rates.

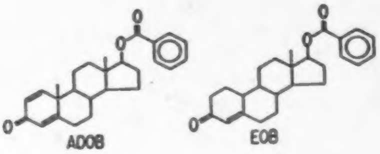


Figure I-19 Structures of molecules containing benzoate and either dienone (in ADOB = androstadiene-3-one-17-ol benzoate) or enone (EOB) groups. In low-temperature glasses the extent and direction of electron transfer between these groups is strongly influenced by solvent polarity.

In a rigid polar solvent (n-pentanol glass at 77K), 97 ± 3% of electrons captured by ADOB are located on the dienone group by our earliest observations at 10^{-7}s. In a somewhat less polar glassy solvent (MTHF), this number drops to 87% at 10^{-7}s, but no change occurs to at least 10^{-2}s. ET kinetics are fast ($<10^{-7}$s) but incomplete. In EOB the direction of ET reverses with solvent polarity: most electrons are on the enone group in pentanol, but most are on the benzoate group in MTHF. The assymetric distributions of electrons are due to fast intramolecular ET reactions since all three groups (enone, dienone and benzoate) react similarly with trapped electrons in both solvents. These observations show that increased solvent polarity can favor the smaller group (the enone in EOB) and can even reverse the direction of ET reactions. The extent of ET is determined by frozen-in distributions of solvation energy. Different arrangements of solvent molecules around otherwise identical ions give different solvation energies. The combination of the distributions of width σ_1 and σ_2 for the two molecular groups give a distribution $P(\Delta E_{12})$ of reaction exothermicities of width $\sigma_{12} = (\sigma_1^2 + \sigma_2^2)^{1/2}$, where $P(\Delta E_{12})$ is the probability of having a given exothermicity, ΔE_{12} as shown in Figure I-20. The extent of reaction is the unshaded area under the $P(E\Delta_{12})$ curve. From the observed extents of reaction, σ_{12} was found to be 0.1eV. This appears to be the first measurement of the distribution of "site energies" for electron transfer, although such distributions have been measured in many cases for optical absorption and emission spectra of molecules.

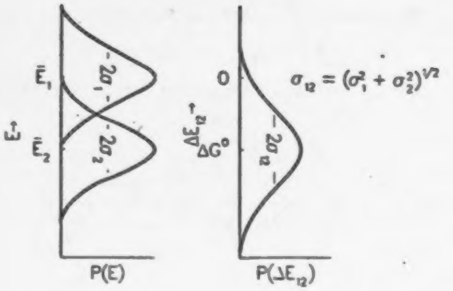


Figure I-20. Probability distributions P(E) for two ions having average redox energies at E_1 and E_2 lead to a distribution of exothermicities, $P(\Delta E_{12})$, for electron transfer between the two types of ions. The extent of reaction measures the widths of the distributions.

(3) Long-Distance ET by Excited Molecules (J. R. Miller, S. Helms, K. Matusak, M. O'Neil)

The reaction of excited electron donors with electron acceptors,

$$D^* + A \longrightarrow D^+ + A^-, \qquad (I-14)$$

leads to quenching of D^* fluorescence in rigid glasses. The quenching radius is maximized at R ≅ 15 Å for reactions of intermediate exothermicity. For these reactions, no temperature dependence was found from 77 to 256K. For more weakly exothermic reactions, giving shorter quenching radii (R = 8-10 Å), quenching was thermally activated over this temperature range. At high exothermicity (ΔG^0 = - 2.0eV) quenching decreased, although no comparable decrease has been seen in many published reports of electron-transfer fluorescence quenching in fluids. The decrease observed here, like the decrease observed in pulse-radiolysis measurements from this laboratory, indicates that electron-transfer theories are correct to predict decreasing rates at large exothermicities. There had been increasing calls to abandon the theories because of disagreements with experiments in fluids. The current results show, instead, that complications arise in fluids and suggest that the "solid-state" arrangement found in photosynthetic reaction centers has important advantages for preventing highly exothermic back reactions in photochemical energy storage.

3.0 Brookhaven National Laboratory

3.1 High Flux Beam Reactor (HFBR)

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

Answer:

A. Neutron Scattering

At the HFBR, the unique properties of slow neutrons are being used to probe magnetism and elementary excitations in condensed matter, and also to determine the structure of biological molecules and materials of basic and technological importance. Experiments to explore the magnetic ordering and the dynamical properties of ordered and disordered materials are being carried out. Gases adsorbed on surfaces as graphite are being studied, and a variety of incommensurate structures produced by electron charge-density waves on lattice instabilities are under investigation.

Systems of potential technological importance, such as framework structures (e.g.,zeolites), ionic conductors and hydrogen in metals are being studied. Neutron scattering is used to establish the structure of a variety of biological molecules. This is an important complement to x-ray scattering, since neutrons are more effective in determining the location of hydrogen atoms, which are a major constituent of living systems.

B. Nuclear Scattering

One of the most powerful techniques for studying the structure of atomic nuclei is that of radiative neutron capture, in which a beam of low energy neutrons from a reactor is allowed to impinge on a target sample containing nuclei of some element. These nuclei capture the neutron to form a new isotope of the same element. This resulting nucleus is formed in an excited state and it must divest itself of the extra energy. It does this by emitting a sequence of γ rays each leaving the nucleus in successively lower states of excitation. By studying these γ rays the nuclear structure (shapes, modes of motion and excitation, interactions of the protons and neutrons within the nucleus) can be unravelled. This technique, usually called (n,γ), is particularly powerful because it populates essentially all all low-lying excited states of the resulting nucleus and thus offers a unique test of modern comprehensive nuclear models that attempt to account, not just for the properties of a few excited modes, but for all of them.

The research program at the HFBR in this field, is the only one of its kind in the United States.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

Answer: With a maximum thermal neutron flux of 1 x 10^{15} neutrons/cm^2-second, the HFBR ranks among the foremost sources of neutrons in the world. There is a cold neutron moderator for producing very slow, long wavelength neutrons, and an on-line isotope generator for production of very short-lived isotopes.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

Answer: There are six triple-axis spectrometers for inelastic scattering, crystallography and experiments with polarized neutron beams. Two double-axis spectrometers are used for diffraction, chemical crystallography and small-angle scattering from biological systems. There is a station for protein crystallography and a small angle scattering facility at the cold neutron moderator.

A variety of ancillary equipment is used to control sample environments. Temperatures from 0.03 K to 1700 K, magnetic fields up to 90 kG and pressures up to 30 kbar are available at many of the experimental stations.

There are two spectrometers for neutron capture studies of nuclear structure, an on-line isotope separation facility and a fast chopper for analysis of resonant capture γ-rays.

Further details may be found in the HFBR handbook, which accompanies this report. (See Question 20 below.)

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer: Some examples of research highlights are:

1. In the field of phase transitions, it is important to understand the effects of competition between different kinds of long range order. This has been explored in a series of experiments on ternary alloys which can display superconductivity and magnetic order. It was shown that superconductivity can coexist with antiferromagnetism but is destroyed by ferromagnetic order. The existence of a novel magnetic state was established.

2. Many features of magnetism in disordered materials which are only just beginning at the HFBR have shown that a weak magnetic field can destroy antiferromagnetism in certain diluted systems. The circumstances in which this takes place and the hitherto unexpected role of long-lived domains has been established. The ideas developed from these experiments will be of importance in understanding the effects of disorder on a wide variety of phase transitions.

3. Lattice instabilities and charge-density waves frequently give rise to a modulation of the underlying lattice. The period of the modulation may have a simple rational relationship to that of the lattice, or it may vary with temperature and pressure, passing through a sequence of incommensurate phases. These phenomena are most effectively explored by means of scattering experiments. At Brookhaven, studies of the phase diagrams and dynamical properties of a variety of such systems--ferroelectrics, insulators and organic metals--coupled with parallel theoretical developments, have led to an understanding of these new phases of matter and have suggested new avenues for research.

Other significant areas of research in condensed matter physics are: structures of surface phases, large-amplitude anharmonic excitations, paramagnetic scattering in itinerant magnets, critical phenomena at magnetic and structural phase transitions, spin glasses, transitions in intercalated systems, mixed valence materials and local modes in hydrides.

In chemical crystallography, highlights have been:

1. The first reported three-dimensional single-crystal structural studies of zeolites, leading to a precise description of the extra-framework ions and water of crystallization.

2. Structure analysis of organometallic compounds, including metal hydrides and compounds exhibiting C-H... metal interactions. These studies provide data on the bonding of hydrogen atoms and organic molecules to transition metals, and are important for problems in catalysis and hydrogen storage.

Other areas of research in chemical crystallography have included ionic conductors, hydrogen in metals, electron charge- and spin-density distributions, high resolution studies of small molecules and determination of the spontaneous polarization in pyroelectrics and ferroelectrics.

There is an extensive program in structural biology carried out in cooperation with university groups. Research highlights in this area are:

1. Determination of molecular weights and shapes
2. Nucleic acid-protein-lipid distribution in large complexes
3. Structural studies of membranes
4. Determination of hydrogen positions in proteins
5. Hydrogen-deuterium exchange studies in proteins
6. Determination of bound water in biomolecules
7. Determination of polymer structures
8. Micelle studies
9. Virus structures

A main thrust of the nuclear structure program at the HFBR has been to map out the structure and symmetries of excited states of nuclei with excitation energies up to 2 MeV. The experimental data have been used to establish and refine the Interacting Boson Approximation (IBA) - a model which incorporates the essential symmetry of Cooper pairs in the nucleus and allows the detailed calculation of collective modes. The IBA is regarded as one of the most significant advances in nuclear structure physics in the past twenty years. Recent work at the HFBR has provided the first evidence for multi-j supersymmetry in nuclei.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: In the Spring of 1981, the cold neutron moderator came into operation. This provides intense beams of very low energy neutrons, which are of growing importance for neutron scattering studies.

During FY 1983, the power of the HFBR was increased from 40 to 60 megawatts.

In FY 1985 there will be installed (a) an intermediate resolution spectrometer for membrane studies and (b) a polarized beam spectrometer for elastic and inelastic scattering studies. The latter has been developed through the U.S.-Japan Cooperative Research Program in Neutron Scattering.

In FY 1984 a pilot facility for slow positron research will be established at the HFBR. It is based upon short-lived high-intensity ^{64}Cu sources produced by neutron irradiation, and with the aid of brightness-enhancement techniques, is designed to give a positron current ten thousand times as large as that obtainable with conventional sources.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer: The following table provides the funding requested.

BROOKHAVEN NATIONAL LABORATORY
HIGH FLUX BEAM REACTOR
(Dollars in Thousands)

BUDGET AUTHORITY

BUDGET PROFILE

		Fiscal Years				
	Source of Funds	1981	1982	1983	Est. 1984	Est. 1985
OPERATIONS	Materials Sciences	$ 4,067[1]	$ 4,700[1]	$ 5,800	$ 6,600	$ 7,800
RESEARCH						
IN-HOUSE	Nuclear Sciences	962	1,135	—	—	—
	Materials Sciences	2,433	2,630	3,243	3,449	3,797
	Chemical Sciences	666	722	381	426	426
	Nuclear Physics	—	—	1,300	826	900
	Environmental R&D	528	606	624	683	727
OUT-OF-HOUSE	Government Agencies*	1,039	1,154	1,268	1,363	1,464
	Private Sources	395	438	487	523	563
TOTAL RESEARCH		$ 6,023	$ 6,685	$ 7,303	$ 7,270	$ 7,877
INVENTORIES	Materials Sciences	$ 47	$ 301	$ 200	$ 353	$ 1,000
CAPITAL EQUIPMENT (INCLUDES CAPITAL FOR OPERATIONS AND RESEARCH)	Materials Sciences	$ 145	$ 175	$ 441	$ 425	$ 555
	Chemical Sciences	50	175	60	113	153
	Nuclear Physics	181	90	90	100	125
	Environmental R&D	150	150	141	32	69
TOTAL CAPITAL		$ 526	$ 590	$ 732	$ 670	$ 902
ARAM	Materials Sciences	$ —	$ 35	$ -	$ 40	$ 500
GPP	High Energy Physics	$ 97	$ 56	$ 66	$ 80	$ 120
IN-HOUSE ENERGY MGMT	Energy Supply R&D	$ —	$ —	$ 285	$ -	$ -
OTHER CONSTRUCTION	Materials Sciences	$ —	$ —	$ -	$ -	$ -

*DOE & OTHERS

[1] See attached.

NOTE: Funding levels above reflect the latest information available from the laboratory, and may vary slightly from information previously provided.

FY 1981 & 1982 HFBR operations were funded through research programs as follows:

	($ in 000's) FY 1981	FY 1982
Nuclear Sciences	$1,123	$1,153
Materials Sciences	1,462	1,763
Chemical Sciences	1,011	1,221
Biological & Environmental	448	543
Irradiations Billed	23	20
	$4,067	$4,700

7. How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?

Answer:

	B/A ($ in 000's)				
	1981	1982	1983	1984	1985
National Science Foundation	259	250	250	250	250
Exxon Corp. (Equip.)	0	0	500	0	0
U.S. - Japan Coop. Prog.	0	0	27	33	40
U.S. - Japan (Equip.)	0	300	400	200	0

8. For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.

Answer:

FTE's	Fiscal Years				
	1981	1982	1983	1984	1985
Operations	46	50	54	60	62
Research	44	47	50	51	51
Total FTE's	90	97	104	111	113

9. What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?

Answer: The utilization of the facility is 95%, based upon 100% operation of beam lines and 50% for the irradiation thimbles.

During FY 1981 to FY 1983, the HFBR operated 24 hours per day for approximately 270 days per year. Allowing for the necessary shutdown periods, during which fuel elements are changed, this constituted full utilization of the facility. The current and projected operating cycle at sixty megawatts allows operation during 290 days per year.

10. For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?

Answer: There have been 1,412 experiments started, continued and completed over the past five years. It would be reasonable to assume that an annual total could be arrived at by dividing the total number by five.

11. What is this facility's user policy?

Answer: The HFBR is a National User Facility; workers from other laboratories are able to carry out experiments there, after peer review of their research program. In the past, there have been different approaches to the implementation of this policy for the different scientific disciplines.

Starting in FY 1984, the Participating Research Team (PRT) system has been adopted for the HFBR. This will provide a unified users policy for the HFBR and the NSLS, where the PRT system is already in effect.

Existing and future spectrometers will be constructed and/or operated by PRT's, organized by discipline, and consisting of members from Brookhaven, universities, industry and other government laboratories. The PRT's are given priority for up to 75% of their spectrometers' operational time. General users are scheduled for PRT spectrometers and for certain instruments designated as general user facilities.

12. **For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?**

    Answer: For the five year period very little reimbursable work has been done at the HFBR. The work that has been performed was for irradiations with a value of less than $20,000 per year.

13. **What is the mechanism by which specific research proposals for experiments at the facility are considered?**

    Answer: In the past, proposals have been received and scheduled, by discipline. A variety of review procedures have been in effect. Under the newly adopted policy, proposals for the formation of Participating Research Teams, and proposals from general users for single experiments or for experimental programs are submitted to the HFBR Program Advisory Committee for review.

14. **How many research proposals have been submitted over the past five years, and how many of these have been approved?**

    Answer: Approximately 1,000 research proposals have been submitted over the past five years and 90 percent of these proposals have been approved.

15. **How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?**

    Answer: Researchers utilizing the HFBR during the past five years from universities total 510.

16. **How many industrial researchers have utilized the facility over the past five years?**

    Answer: Researchers utilizing the HFBR during the past five years from industry total 65.

17. **How many researchers from foreign institutions have utilized the facility over the past five years?**

    Answer: Researchers utilizing the HFBR during the past five years from foreign countries total 275.

18. **How many researchers from other agencies have utilized the facility over the past five years?**

    Answer: Researchers utilizing the HFBR during the past five years from other agencies total 85.

19. **What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?**

    Answer: There are many potential future development possibilities for the existing High Flux Beam Reactor, but there are currently no specific plans to undertake any of them beyond the construction activities identified in the FY 1985 budget request.

20. **Please provide a copy of the facility's latest annual report.**

    Answer: There is no annual report for this facility. A copy of the HFBR handbook is attached. **(Note: Excerpts from this handbook follow.)**

BNL 24182
REVISED

HFBR HANDBOOK

AUGUST 1983

INFORMAL REPORT

BROOKHAVEN NATIONAL LABORATORY
UPTON, LONG ISLAND, NEW YORK 11973
ASSOCIATED UNIVERSITIES, INC.
UNDER CONTRACT NO. DE-AC02-76CH00016 WITH THE
UNITED STATES DEPARTMENT OF ENERGY

PREFACE

This manual is intended primarily to acquaint outside users and new Brookhaven staff members with the research facilities available at the HFBR. In addition to describing the beam lines and major instruments, general information is also provided on the reactor and on services available at the Laboratory. We are indebted to members of the user groups in the Brookhaven Department of Physics, Chemistry, and Biology for providing the information from which the manual was assembled. We would also like to acknowledge, in particular, the valuable assistance of F.T. Langdon for coordinating the preparation of figures for the experimental facilities.

The Editors
S. Shapiro, D.C. Rorer,
and H. Kuper

I. The High Flux Beam Research Reactor

Since their discovery by Sir James Chadwick in 1932, neutrons have been studied not only in themselves, but have provided an extremely powerful tool for studying matter on the nuclear, atomic, and molecular levels as well. Neutrons have been used as probes by nuclear and solid state physicists, chemists, and most recently, by biologists. As techniques for using neutrons have developed in these various disciplines, there has been an accompanying need for higher levels of neutron flux in order to carry out more complex and sophisticated experiments. The Brookhaven High Flux Beam Reactor (HFBR) was designed to meet this need, providing a total flux of 2.4×10^{15} neutrons/cm^2-sec at a power of 60 megawatts.

The HFBR first achieved criticality on October 31, 1965, approximately four years after construction began, and became available for general experimental use at full power several months later. The initial construction cost of the HFBR was $12.5 million, and its current annual operating cost is approximately $6.1 million (including associated overhead cost distributions).

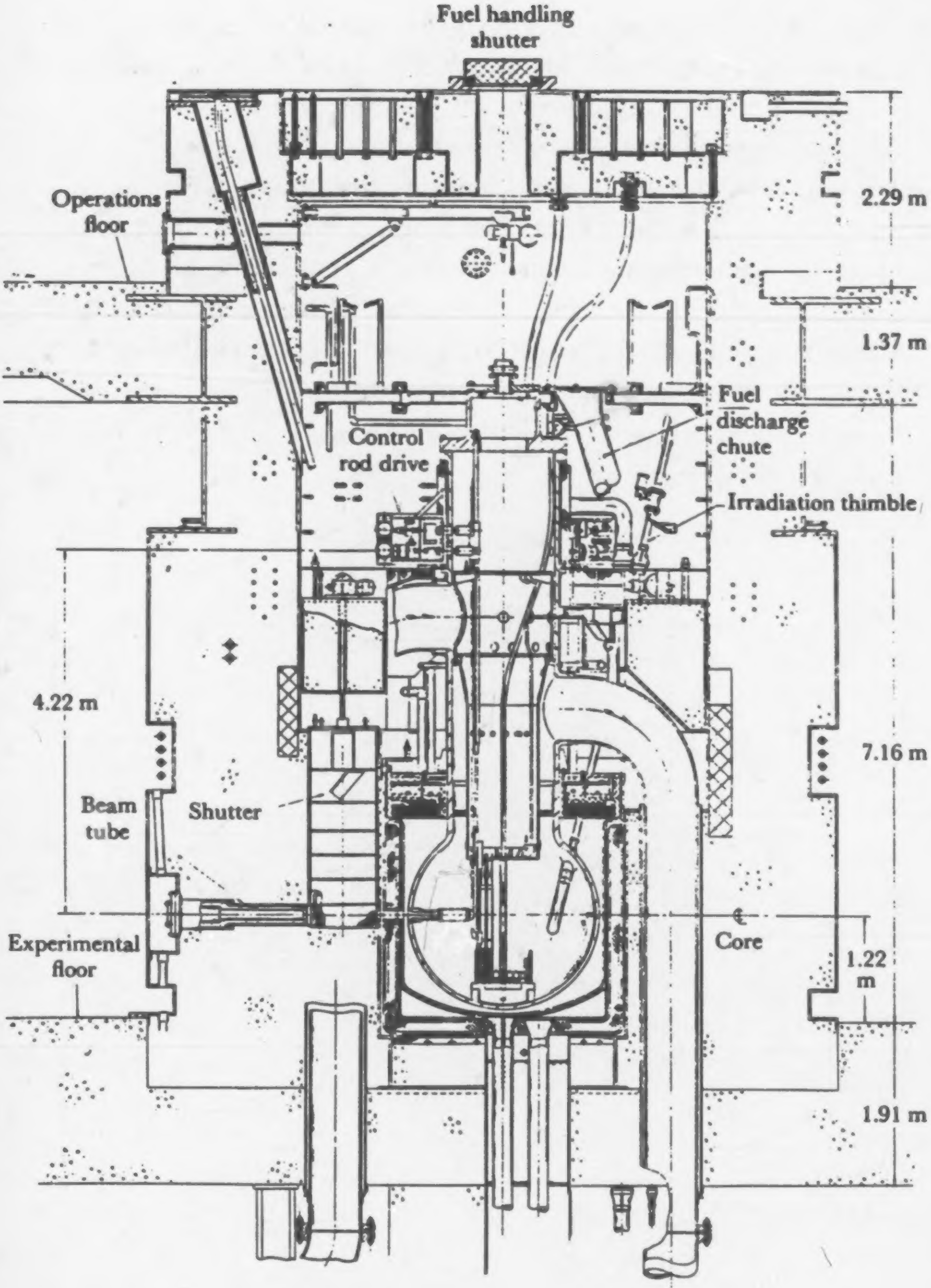
GENERAL DESCRIPTION OF THE REACTOR

The HFBR uses highly enriched U-235 fuel and a heavy water moderator to sustain a controlled nuclear reaction. The core consists of 28 elements, each containing 18 curved fuel plates (of the Materials Testing Reactor Type). In each plate U_3O_8 powder is mixed with aluminum powder to form a cermet core, which is encased in aluminum cladding. The cladding acts as a barrier or containment for the highly radioactive isotopes formed as fission products during the chain reaction.

The fuel elements are placed in a roughly cylindrical arrangement inside a spherical-shaped aluminum reactor vessel. The core is approximately 53 cm high and 48 cm in diameter, has an active volume of about 97 liters and contains a maximum of 9.8 kilograms of U-235. The D_2O moderator is pumped downward through the spaces between the fuel element plates at a pressure of 1.4×10^6 pascals, carrying away the 60 megawatts of thermal energy developed in the core during normal reactor operation. The D_2O is circulated through a pair of heat exchangers where the heat is transferred to an H_2O secondary loop which dissipates the heat into the air through a set of cooling towers.

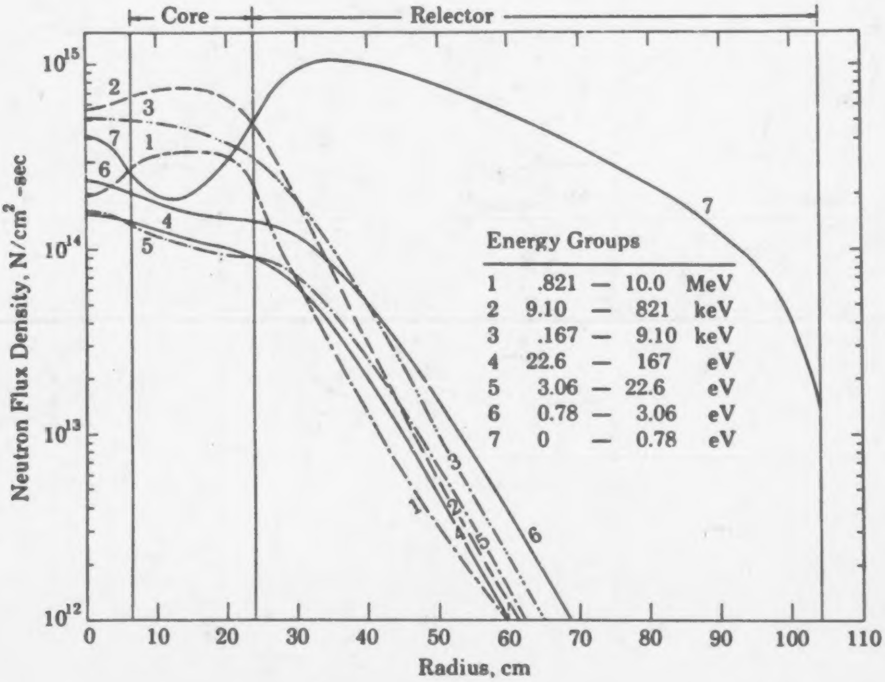
Outside the reactor vessel is a water-cooled thermal shield of steel and lead 23 cm thick. This secondary vessel protects the surrounding outer shield from excessive heating by radiation from the reactor and provides containment to keep the core covered with heavy water in the event of a leak in the reactor vessel. An outer shield, known as the biological shield, protects the reactor operators and experimenters from the radiation produced in the reactor. The biological shield, which has a minimum thickness of 2.4 meters, is a mixture of heavy concrete and steel punchings.

In contrast to most reactors, which are designed to minimize the escape of neutrons from the core, the HFBR has been expressly designed to maximize the number of neutrons available in external beams. This is accomplished through the choice of coolant material and core configuration. Heavy water, rather than light water, has been selected as the coolant and moderator in this reactor. The volume of D_2O flowing through the core to cool the fuel elements does not provide sufficient moderation to thermalize all the neutrons


Fuel handling shutter
Operations floor
2.29 m
1.37 m
Fuel discharge chute
Control rod drive
Irradiation thimble
4.22 m
7.16 m
Beam tube
Shutter
Experimental floor
Core
1.22 m
1.91 m

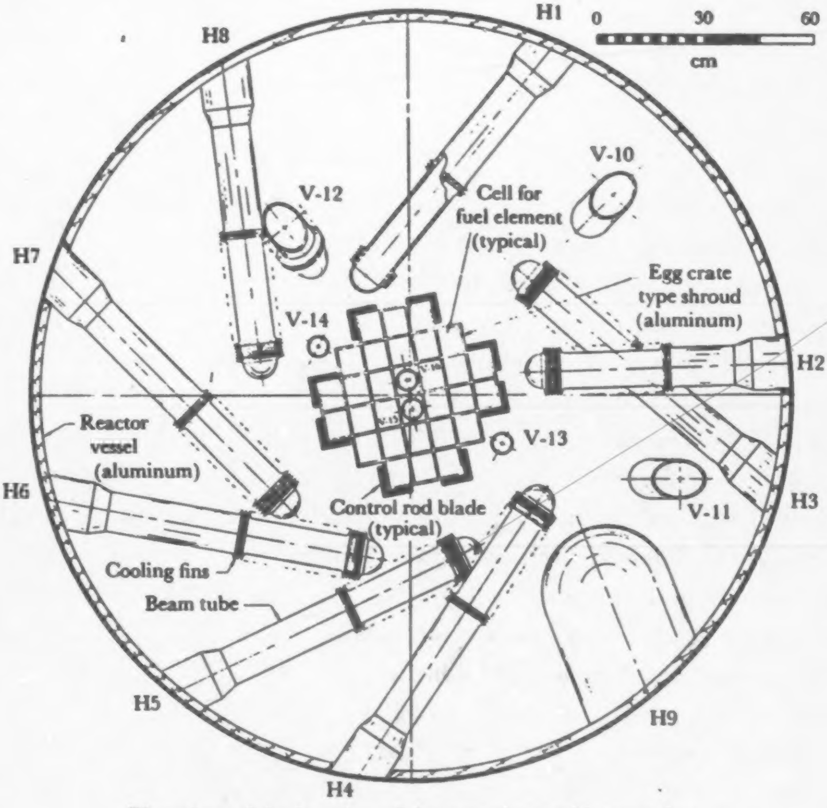
Elevation of the reactor vessel and shielding, showing a typical beam tube, shutter, and thimble.

within the core. A large number of fast and epithermal neutrons thus escape from the region of the fuel and are subsequently moderated in the large volume of D_2O reflector surrounding the core. Some of the resulting thermal neutrons are reflected back into the core where they help to sustain the nuclear chain reaction. This choice of materials and configuration results in a unique neutron distribution in which the useful thermal neutron population peaks in the reflector, where the neutrons are directly accessible to the beam tubes. The higher energy neutrons, which are normally not desirable in the beams, are greatest in population within the core. Power density is peaked at the periphery rather than at the center of the core as in most other reactors.



Calculated neutron flux distributions as a function of radial distance from the center of the core.

Sixteen control rods containing dysprosium and europium oxides act as neutron "poisons" to absorb thermal neutrons and control the rate at which the nuclear reaction takes place. These rods are located just outside the core and are arranged into two groups, a main bank which can be raised above the core, and an auxiliary bank which can be lowered below the core. Shutdown of the chain reaction is accomplished by masking the core from the return of thermal neutrons from the reflector by covering the sides of the core with the control rod blades. During normal operation, the neutron flux is maintained constant at the core midplane by withdrawing the control rods approximately symmetrically from the top and bottom of the core as fuel burnup progresses.


H1
0
30
60
cm
H8
V-10
V-12
Cell for
fuel element
(typical)
H7
Egg crate
type shroud
(aluminum)
V-14
H2
V-16
V-15
Reactor
vessel
(aluminum)
V-13
H6
Control rod blade
(typical)
V-11
H3
Cooling fins
Beam tube
H5
H9
H4

Plan view of the location of the experimental beam tubes and irradiation facilities within the reactor vessel.

HFBR Statistics

Reactor power	60 million watts
Total fast neutron flux, fuel region	2.4×10^{15} n/cm^2-sec
Maximum thermal flux, reflector	1.05×10^{15} n/cm^2-sec
Active core volume	97 liters
Active height of core	52.7 cm
Diameter of core (equivalent cylinder)	47.8 cm
Number of fuel elements in core	28
Dimensions of fuel element	
Cross section (fuel plates)	8.113 × 7.163 cm
Length of 2 outer plates	58.4 cm
Length of 18 inner fuel plates	52.7 cm
Total length of fuel element	154.4 cm
Uranium-235 content of fuel element	351 g
Total uranium-235 loading	9.8 kg
Reactor coolant	heavy water (D_2O)
Total coolant flow rate	1150 liters/sec
Maximum operating coolant pressure	1.72×10^6 pascals
Maximum operating inlet coolant temperature	65° C
Maximum temperature at fuel element surface	≈175°C
Number of control rods	16
Dimensions of control rod cross section (rods are right angle shape)	7.6 × 7.6 × 1.78 cm
Length of main rods	102.9 cm
Length of auxiliary rods	31.8 cm
Neutron absorber in rods	Dy_2O_3 and Eu_2O_3
Diameter of spherical portion of reactor vessel	208.3 cm
Diameter of neck of reactor	121.9 cm
Thickness of thermal shield (lead and steel)	22.9 cm
Minimum thickness of biological shield (heavy concrete)	243.8 cm

The HFBR is operated 24 hours per day for a period of either 14 or 24 days, depending on the number of fuel elements which are replaced with new fuel during the shutdown at the end of each operating cycle. If seven elements are replaced, the operating cycle will last 14 days, while replacement of 14 elements results in a 24-day cycle. The refueling shutdown normally lasts for a period of 3 to 6 days, varying with the amount of maintenance and surveillance testing which must be done.

For safety reasons, all nuclear reactors are designed with a negative temperature coefficient of reactivity, so that any power surges which might occur will be self-limiting due to the automatic decrease in reactivity as the reactor heats up. This safety feature has an important effect on the maximum length of the operating cycle which can be obtained at the HFBR. During the summer months the efficiency of the cooling towers can vary over a wide range in a short time, depending on air temperature and humidity. The corresponding changes in reactor coolant temperature produce changes in the reactivity which become especially significant near the end of the fuel cycle, when there is little excess reactivity to spare. Negative reactivity effects under such conditions can sometimes result in insufficient reactivity being available to sustain the chain reaction and can cause a premature shutdown, shortening the operating cycle by as much as one day. Conversely, cold winter days coinciding with the end of the fuel cycle can prolong the cycle.

THE CONFINEMENT BUILDING

The reactor, its auxiliary equipment, and its experimental facilities are contained in a welded steel hemisphere 53.6 meters in diameter. While the reactor is in operation the air pressure inside the building is kept slightly lower than the atmospheric pressure outside to insure that any air leakage is inward rather than outward. Access to the building is provided by a system of air locks. This building provides the final confinement barrier against the escape of radioactive material into the environment. All ventilation air leaving the building is processed through high efficiency particulate filters and charcoal absorbers before being discharged from a 100 meter stack.

There are three basic floor levels in the building. The bottom floor is known as the Equipment Level. The main features of this level are a shielded cell in the center of the floor, containing the primary coolant system pumps and heat exchangers, and the fuel storage canal. The highly radioactive spent fuel elements are discharged into the canal through a chute passing down from the top of the reactor vessel through the concrete shielding. The canal presently has storage capacity for as many as 833 elements. The canal is 6 meters deep for most of its length, with a 9-meter deep pit at the end of the fuel discharge chute. The spent fuel elements are stored under the shielding water of the canal until most of the radioactivity has died away and they can be shipped off site to a fuel reprocessing plant for recovery of the unused uranium-235.

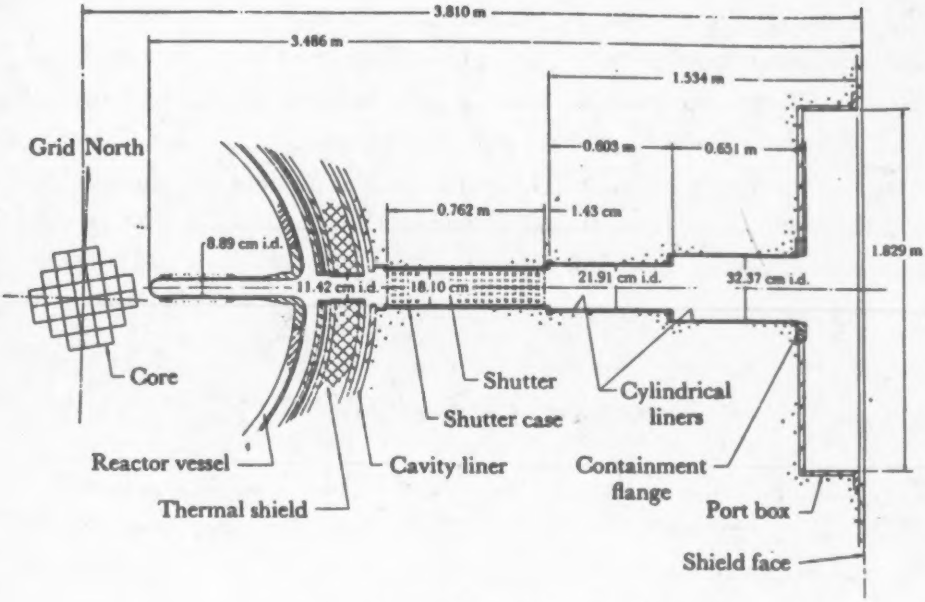
Other auxiliary equipment located on this floor includes heat exchangers and pumps for the coolant for the thermal shield and the biological shield, purification systems for the D_2O coolant and canal water, as well as the equipment supplying the building with electrical power, steam, hot water, and compressed air.

The Experimental Area occupies the middle floor. The reactor is located in the center of the floor, with its nine horizontal beam ports surrounded by massive shielding and complex equipment for external beam experiments. Laboratories, computer equipment rooms, and a health physics office are also located on this floor level. A radial 18000 kg traveling beam crane serves this area. Truck and fork lift access is provided by two separate air locks. A balcony above the main floor is available for observation and accommodates washrooms, offices, and air conditioning equipment. A machine shop is located adjacent to this level outside the confinement building.

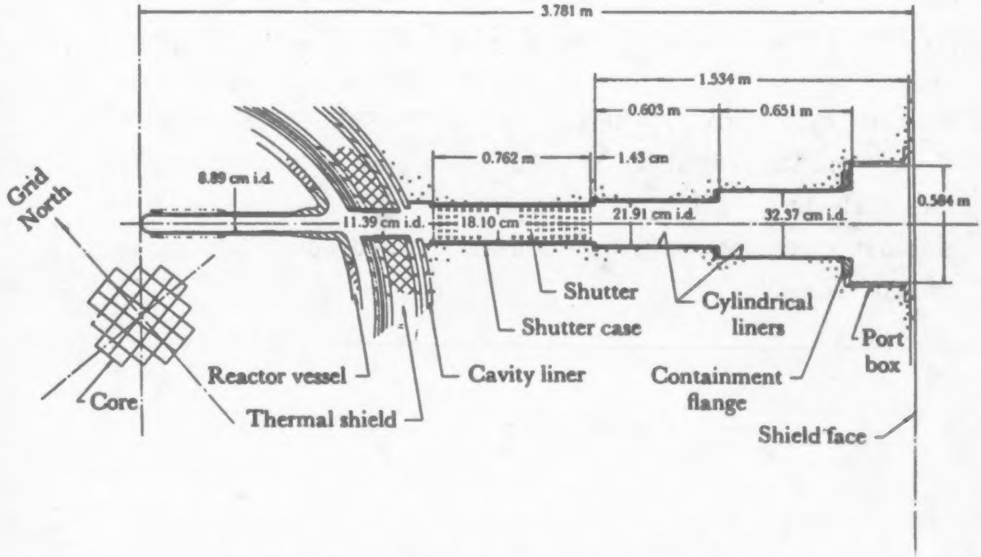
The Operations Area is on the top floor of the building. The reactor shielding structure rises 2.3 meters above floor level in the center of the area. The reactor control room, the pumps and heat exchangers for the cooling system for the vertical irradiation tubes, the D_2O storage tank for the primary coolant system, offices, work rooms, and the fuel storage vault are located on this floor. An 18000 kg overhead crane services the reactor top and the adjacent area in which replacement of spent fuel elements with new ones takes place.

BEAM TUBE DESIGN

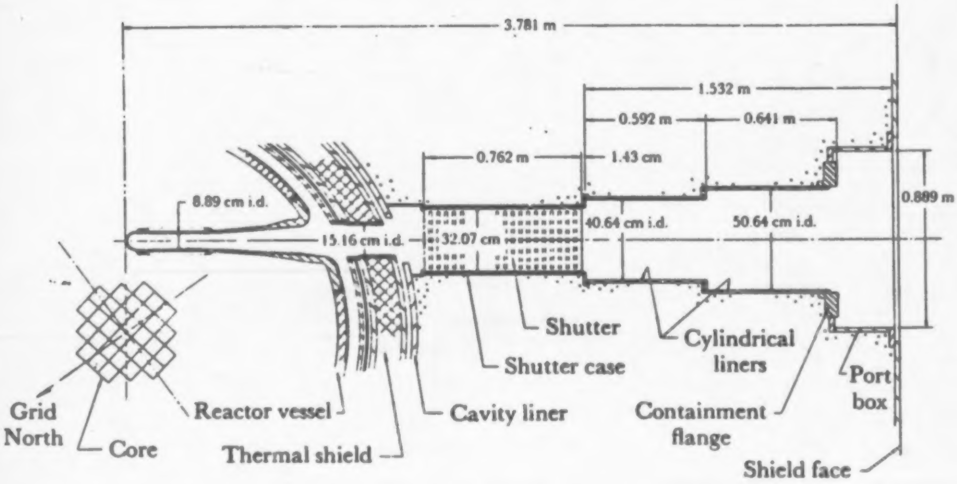
The accompanying figures in this Section provide information which may be helpful to users in understanding the capabilities of the various instruments described in Section IV, or in planning their experiments if some new type of installation is contemplated. Several types of beam tubes were incorporated into the HFBR design. H2 is the only tube which "looks" directly at the core; it was designed specifically for nuclear studies employing fast neutrons. H3 is typical of the single thermal neutron tubes, used also at H1, H5, H7, and H8. Dual thermal tubes are used at H4 and H6, facilitating development of two beam lines at each of these ports. H9 is a special large diameter tube which was designed to accommodate a cold neutron moderator. The remaining figure shows a more-or-less typical section in elevation of a beam tube penetration through the biological shield into the reactor vessel, along with a typical double-axis spectrometer installation.


3.810 m
3.486 m
1.534 m
0.603 m
0.651 m
0.762 m
1.43 cm
1.829 m
Grid North
8.89 cm i.d.
11.42 cm i.d.
18.10 cm
21.91 cm i.d.
32.37 cm i.d.
Core
Shutter
Shutter case
Cylindrical liners
Reactor vessel
Cavity liner
Containment flange
Thermal shield
Port box
Shield face

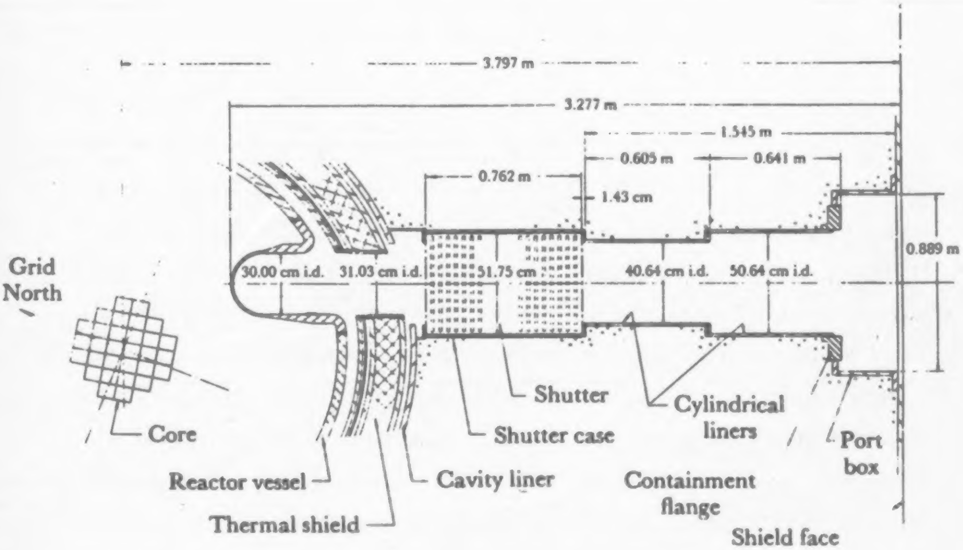
Plan of HFBR beam tube H2.


3.781 m
1.534 m
0.603 m
0.651 m
0.762 m
1.43 cm
0.584 m
Grid North
8.89 cm i.d.
11.39 cm i.d.
18.10 cm
21.91 cm i.d.
32.37 cm i.d.
Shutter
Shutter case
Cylindrical liners
Port box
Reactor vessel
Cavity liner
Containment flange
Core
Thermal shield
Shield face

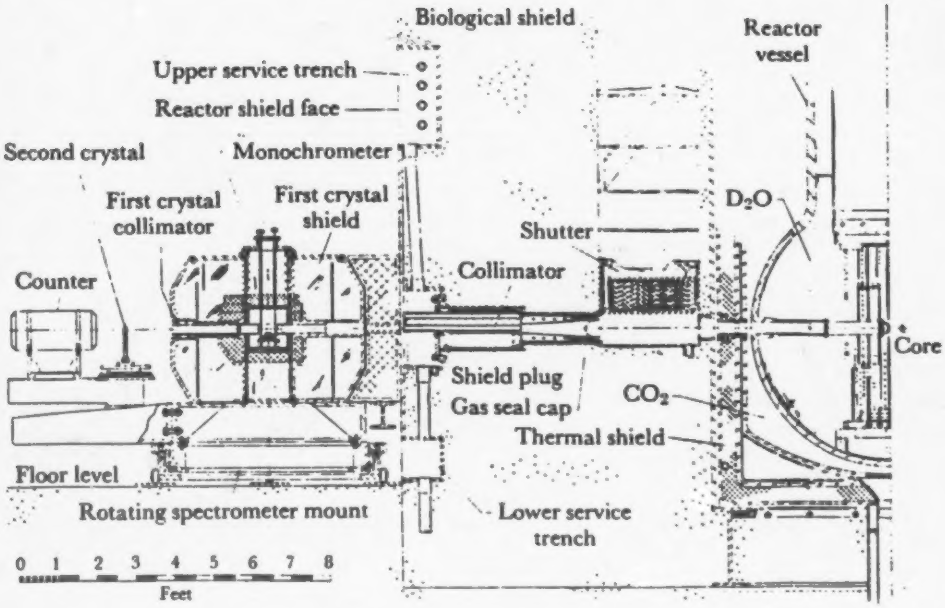
Plan of HFBR beam tube H3 typical of thermal tubes.


3.781 m
1.532 m
0.592 m
0.641 m
0.762 m
1.43 cm
8.89 cm i.d.
15.16 cm i.d.
32.07 cm
40.64 cm i.d.
50.64 cm i.d.
0.889 m
Shutter
Shutter case
Cylindrical liners
Port box
Grid North
Core
Reactor vessel
Thermal shield
Cavity liner
Containment flange
Shield face

Plan of HFBR beam tube H4 typical of dual thermal tubes.


3.797 m
3.277 m
1.545 m
0.605 m
0.641 m
0.762 m
1.43 cm
0.889 m
Grid North
30.00 cm i.d.
31.03 cm i.d.
51.75 cm
40.64 cm i.d.
50.64 cm i.d.
Shutter
Shutter case
Cylindrical liners
Port box
Core
Reactor vessel
Thermal shield
Cavity liner
Containment flange
Shield face

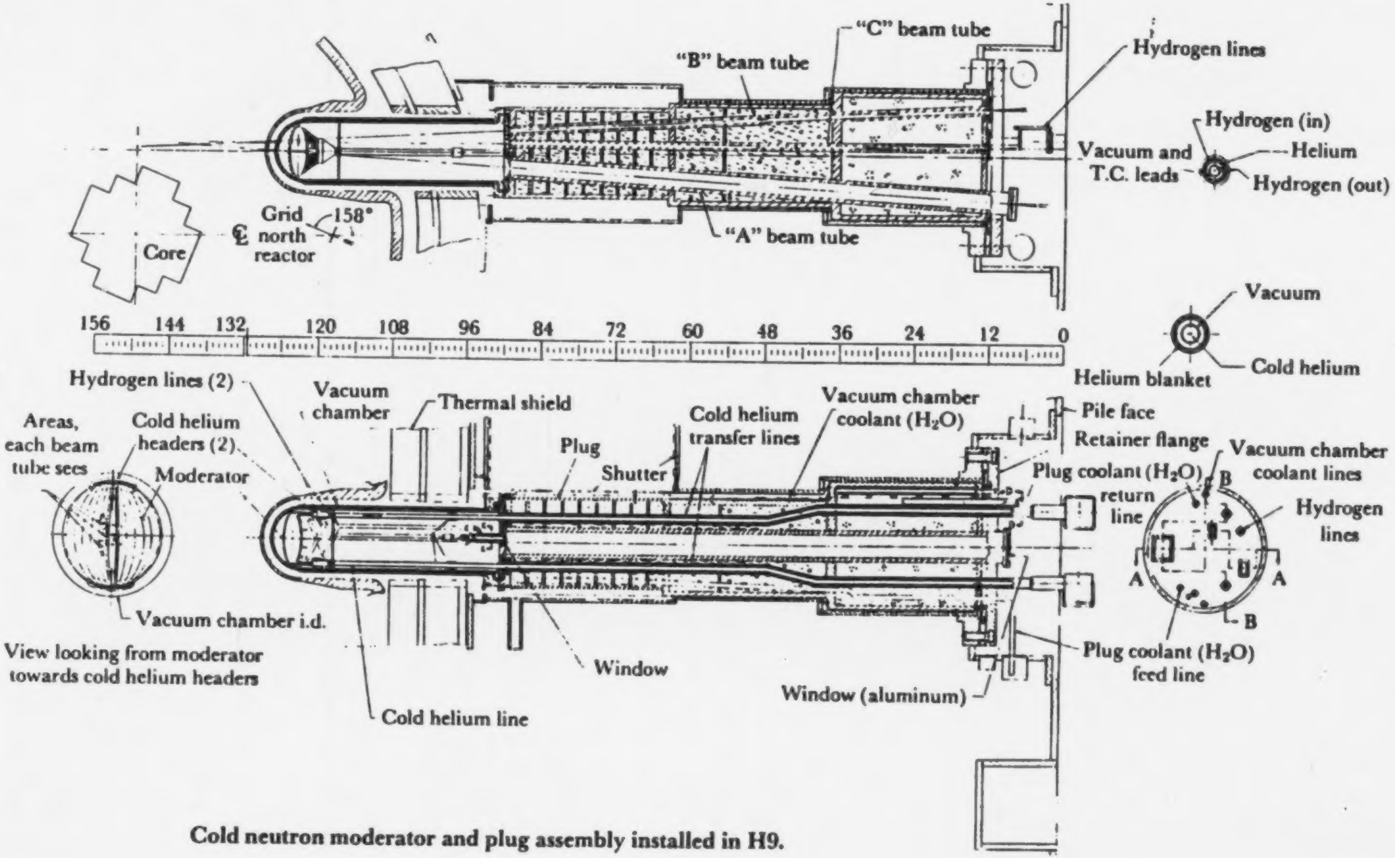
Plan of HFBR beam tube H9.


Biological shield
Reactor vessel
Upper service trench
Reactor shield face
Second crystal
Monochrometer
First crystal collimator
First crystal shield
D2O
Shutter
Counter
Collimator
Core
Shield plug
Gas seal cap
CO2
Thermal shield
Floor level
Rotating spectrometer mount
Lower service trench
0 1 2 3 4 5 6 7 8
Feet

Elevation of double-axis spectrometer and beam tube (typical).

COLD NEUTRON MODERATOR

To provide intense beams of very low energy neutrons ($\leq$5 meV), a liquid hydrogen moderator system has been installed in the H9 beam thimble. The moderator chamber contains 1.4 liters of liquid hydrogen and is located near the inner end of the thimble as shown in the accompanying figure. Circulating cold helium gas from an external refrigerator maintains the hydrogen at a temperature of 19K. Neutrons from the surrounding heavy water blanket are moderated by scattering processes within the cold hydrogen, thus shifting the spectral distribution of the emerging beam towards lower energies. In operation the system serves as a cold neutron source for three separate beams, designated as A, B, and C on the accompanying figure. The experimental stations for these beams are described under Experimental Beam Facilities.


"C" beam tube
"B" beam tube
Hydrogen lines
Hydrogen (in)
Helium
Hydrogen (out)
Vacuum and
T.C. leads
Grid
158°
℄ north
reactor
Core
"A" beam tube
Vacuum
Cold helium
Helium blanket
156
144
132
120
108
96
84
72
60
48
36
24
12
0
Hydrogen lines (2)
Vacuum
chamber
Thermal shield
Areas,
each beam
tube sees
Cold helium
headers (2)
Moderator
Plug
Shutter
Cold helium
transfer lines
Vacuum chamber
coolant (H2O)
Pile face
Retainer flange
Plug coolant (H2O)
return
line
Vacuum chamber
coolant lines
Hydrogen
lines
B
A
A
B
Vacuum chamber i.d.
View looking from moderator
towards cold helium headers
Window
Cold helium line
Window (aluminum)
Plug coolant (H2O)
feed line

Cold neutron moderator and plug assembly installed in H9.

II. Safety at the HFBR

The HFBR has achieved an outstanding safety record over more than 17 years of operation. This has been accomplished through careful design, planning, and review, combined with diligence in observing appropriate safety procedures. Such an achievement has been possible only through the continued cooperation of all HFBR users and operating personnel. For the sake of his or her own safety, as well as that of others, it is important for everyone working at this facility to respect and observe the safety guidelines presented in this section.

USE OF THE CONFINEMENT BUILDING

The HFBR confinement building is a restricted access area. All visitors during normal working hours must be accompanied by a person on the approved access list for the HFBR. Admission of visitors at times other than normal working hours may be arranged through the Reactor Division. A person may be placed on the access list with the recommendation of his Department Chairman and only after successful completion of a training and familiarization program given by the Heath Physics Group. Training and access information can be obtained by calling extension 4432.

Because of the possibility of exposure to radiation and contamination with radioactive material, all persons entering the confinement building are required to wear film badges. All material and equipment to be removed from the building must first be checked by the Health Physics Group for possible radioactive contamination.

The closed atmosphere of the confinement building dictates that strict precautions be observed with regard to hazardous materials in the building.

1. Toxic and flammable materials must be in safety cans which identify material stored within.

2. Toxic and flammable materials must be reported to Research Coordination (Ext. 4436), who will inquire as to the need, and obtain safety recommendations.

3. Other materials normally considered to be of minor toxicity or flammability must be examined closely if large quantities are required. Examples of such materials are: oil, grease, paraffin, alkali metals, compressed gases, and cryogenic materials.

4. Any requirement to bring explosive gases into the building must be cleared with Research Coordination for appropriate safety recommendations. Examples of some explosive gases are: H_2, O_2, acetylene.

5. Flammable materials, such as paper cartons, excelsior, and computer printouts, must not be allowed to accumulate.

6. Please refer to the BNL Safety Manual or check with Research Coordination to determine the possible hazardous nature of unfamiliar materials.

7. Elemental mercury is strictly banned from the confinement building because of its possible interaction with aluminum reactor components. The use of mercury compounds should be reviewed by Research Coordination before such compounds are brought into the confinement building.

ACTIONS IN CASE OF HFBR EMERGENCIES

Actions and responsibilities of an individual on becoming aware of an emergency in the HFBR are:

1. Sound the alarm, and summon assistance so that personal injuries and property losses may be held to a minimum.

2. Be familiar with the location and method of activation of manual alarms in his work vicinity.

3. Take emergency action within the scope of his training, to control or limit an emergency in his work vicinity, but avoid exposure to undue risks.

4. On hearing an **Emergency Signal** do the following:

(a) On hearing a **Warning Signal** (continous ringing of HFBR fire bells), **each person in HFBR**, who is not a member of the HFBR Emergency Forces, **shall leave HFBR by the nearest exit**, and shall proceed directly to the HFBR Lobby. Each person shall be alert for further instructions given over the HFBR Public Address System, or by his Supervisor. Supplementary instruction will also normally be directed to the HFBR Emergency Forces over the HFBR Public Address System, or by other means.

(b) On hearing an **Evacuation Signal** (intermittent ringing of the HFBR fire bells), **each person in the HFBR shall leave the building by the nearest exit**, and shall proceed directly to the HFBR Lobby. The only exceptions are:

i. Persons who are in a position to save a life, or to take other vital emergency action enroute to the exit, without undue hazard to themselves;

ii. Persons receiving other specific instructions at the time from the Reactor Shift Supervisor or HFBR Local Emergency Coordinator.

SAFETY REQUIREMENTS FOR EXPERIMENTS

Safety is a line responsibility from the Director of the Laboratory to Department Chairmen. Each experimenter at the HFBR is directly responsible to the Chairman of the Department with which he is associated to conduct his experiment in accordance with prevailing safety regulations. In general, the experimenter has the prime responsibility for planning, designing, fabrication, testing, operation, maintenance, and ultimate disposal of all equipment required exclusively for his experiment. The experimenter is responsible for conforming to appropriate safety standards and for furnishing all information required for safety review by others.

It is the responsibility of the Research Coordinator to work with the experimenters to assure that the HFBR facilities are used to the best advantage and in such a manner as to guarantee the safety of the reactor. The Coordinator will aid the experimenters in obtaining safety approval for their proposed experiments, seeking expert opinion where necessary to substantiate recommendations made to the RCES Committee. For this purpose the Coordinator will generally call upon an Experiments Review Team consisting of representatives from the Reactor Operations Group, Safety and Environmental Protection, and others from the Reactor Division who are familiar with experimental facilities and reactor characteristics.

In general, experiments to be conducted at the HFBR shall be designed and operated in such a manner that:

1. The safety of personnel working in the area is not compromised.
2. Reactor safety can be maintained under all credible conditions created by the experiment (whether normal or abnormal), such that the reactor is not damaged and radioactive releases to the environment are always kept below acceptable limits.
3. Each experiment does not interfere with the operation of any of the others.
4. A preplanned procedure exists for decommissioning each experiment and removing the equipment from the reactor building.

Experiments in beam tubes, irradiation thimbles or elsewhere around the reactor, which potentially could exceed the envelope of reviewed conditions discussed below, or which might present new and unique hazards, will be regarded as "unreviewed hazards." Under the general terms of the prime contract between Associated Universities, Inc. and DOE, and in accordance with pertinent sections of the DOE Manual, such "unreviewed hazards" must be referred to DOE for concurrence before they are permitted at the HFBR. All types of experiments that have been placed in and around the reactor have been reviewed by the BNL Reactor and Critical

Experiments Safety Committee (RCESC), and each new experiment proposed which falls outside the envelope of conditions previously approved will also be reviewed by the Safety Committee. The DOE Brookhaven Office is kept informed on a continuous basis of the experimental program and of the reviews and actions of RCESC.

In-pile Experiments and Equipment

The safety limits on experiments to be inserted into the reactor vessel experimental facilities (beam tubes and irradiation thimbles) are based upon two essential considerations. The first of these is that the maximum reactivity associated with any material to be inserted or removed from the reactor must not be so large that the instantaneous insertion or removal of the material could cause a nuclear transient which would damage the reactor. The second basic consideration is that all experiments to be inserted into the reactor vessel experimental facilities must be of such a nature and constructed in such a way that in no circumstances will the containing beam tube or thimble in the vessel be damaged.

Out-of-pile Experiments and Equipment

With regard to reactor safety limitations on beam experiments, the placing of radiators (scattering blocks) or sample scatterers in the vessel beam tubes is subject to the limitations imposed above. The experimental apparatus placed at the beam ports is subject to the same process of review and testing as are experiments which are placed in the reactor. For example, experimental equipment containing cryogenic or high pressure components must be reviewed by the Safety and Environmental Protection Division. Equipment containing rotating machinery must be extensively tested at above maximum operating speeds for long periods of time to establish the safety of the design. In all cases, the orientation of the rotating equipment to be used outside the shield must be such that failure of the rotor would not direct fragments into beam ports.

Any experiments which contemplate the use of potentially explosive materials, such as hydrogen, in or near the beam ports are subject to the same program of testing as for explosive materials in the vessel thimbles. That is, suitable containment for the explosive or reactive material shall be provided and must be proof-tested by actual experiments in which the maximum possible energy release inside the containing vessel was accomplished.

III. HFBR User Policy

The facilities described in this handbook are open to the general scientific community. No charges will be imposed for their use unless the research is of a proprietary nature, in which case a full cost recovery fee will be charged for the amount of beam time used for the proprietary research. Beam time can be applied for by submitting a research proposal, which will be judged according to scientific merit by the Program Review Committee. For more details contact D. Rorer or S.M. Shapiro.

IV. Experimental Beam Facilities

The instruments available at the HFBR have been developed to cover a wide range of scientific studies. Figure 1 shows a schematic floor layout of the various beam ports, H1 through H9, and the basic experimental installations at each port. The latter may be classified according to their main use:

Nuclear Physics

H1-A H1-B H2

Inelastic Scattering

H4-M H7 H9-A (cold neutrons)
H5 H8

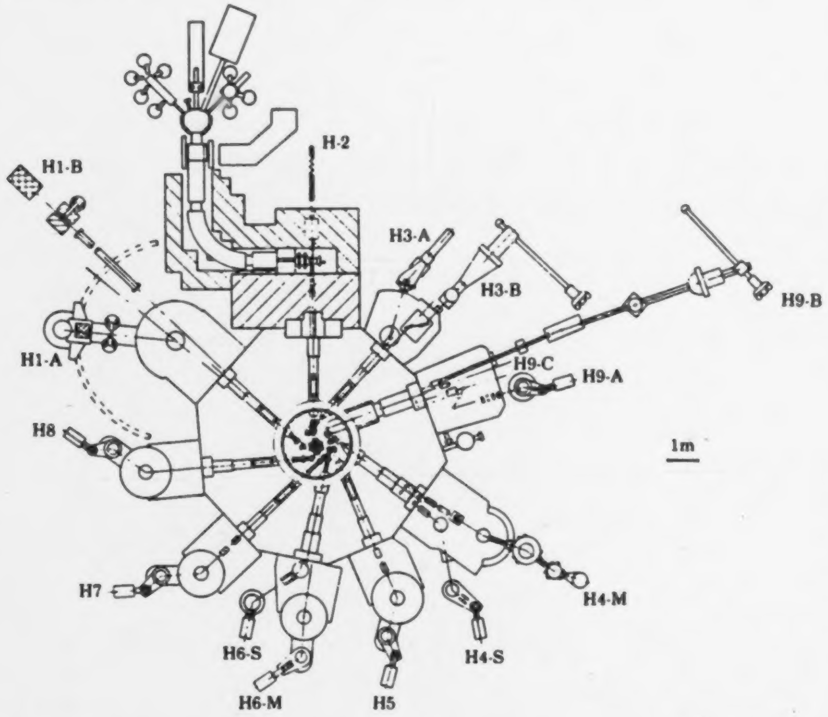
Neutron Diffraction

H4-S (also small angle scattering)
H6-M
H6-S

Biological Structure Studies

H3-A
H3-B
H9-B (cold neutrons)

Details on these experimental stations are given in the subsections which follow.



Schematic plan of spectrometers installed on the experimental level of the HFBR.

H1-A SPECTROMETER (NUCLEAR PHYSICS)

H1 is a tangential beam of exceptional quality featuring high flux and low γ-ray backgrounds. The thimble terminates about 14 cm from the core center. Two beams are extracted from the H1 beam plug. H1-A provides a neutron beam whose properties can be varied to accommodate experiments in several different areas of nuclear physics. Two types of beams are available:

1. A monochromatic beam obtained by Bragg diffraction from several crystals.

2. A high quality thermal beam obtained by filtering the reactor spectrum through crystalline quartz.

H1-A Station Parameters

Monochromators/ Filters	Energy Range	Beam Size	Intensity (E=1.0 eV)
Be($10\bar{1}1$)	0.025—25 eV	2.5×2.5 cm^2	2.2×10^5 n/cm^2-sec
Quartz Filter (58 cm)	Thermal	1.27 cm diam	1.5×10^8 n/sec

Collimation: 3.6 minutes
Angular Range: 0—90°

Detectors: Neutron—BF$_3$; γ-ray—Ge(Li) and multi-Ge (angular correlation)

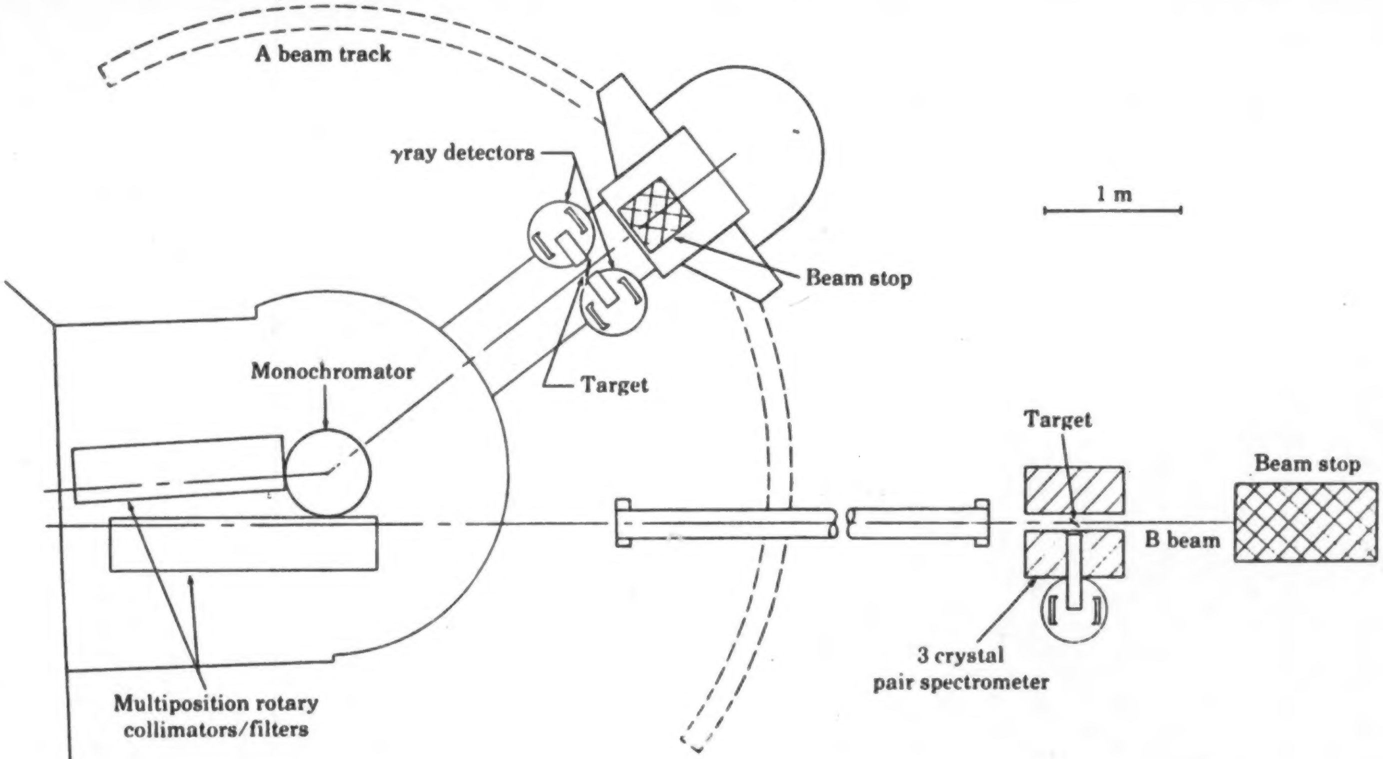
H1-B SPECTROMETER (NUCLEAR PHYSICS)

At H1-B, a flexible external sample facility offers sources for capture studies in the slow neutron, eV, and keV range. Filters for tailoring the beam are contained in a 4-position rotary collimator external to the reactor shield. A set of easily modified filters can be rapidly interchanged so as to span a broad range of neutron energies in a study of a single nuclide. A 3-crystal pair spectrometer is used to detect primary γ-rays from (n,γ) experiments using filtered beams at thermal, 2 keV, and 24 keV with an efficiency of about 3% relative to a 7.6×7.6 cm^2 NaI standard detector. Data are routed into a PDP 11/40 computer and further analyzed using the computer facilities described under beam line H2.

H1-B Station Parameters

Filter	Beam Energy	Width (FWHM)	Size (cm)	Intensity (n/sec)	Purity (%)
22.86 cm Fe 36.20 cm Al 6.35 cm S	24.3 keV	2.0 keV	7.27×2.8	1.4×10^7	98
68.58 cm ^{56}Fe (98.87%)	24.3 keV	1.0 keV	7.27×2.8	1.5×10^8	80
30.48 cm ^{56}Fe 17.78 cm Al	24.3 keV	1.7 keV	7.27×2.8	4.20×10^7	95
71.1 cm Sc	2.0 keV	0.9 keV	7.27×2.8	7.1×10^7	70
Bi single crystal	thermal	Maxwellian	$<7.27\times2.8$ (variable)	$\sim10^9$	

Detector: 3-crystal pair spectrometer


A beam track
γray detectors
Beam stop
1 m
Monochromator
Target
Target
Beam stop
B beam
3 crystal
pair spectrometer
Multiposition rotary
collimators/filters

Schematic plan of spectrometers installed at H1.

H2 TRISTAN MASS SEPARATOR (NUCLEAR PHYSICS)

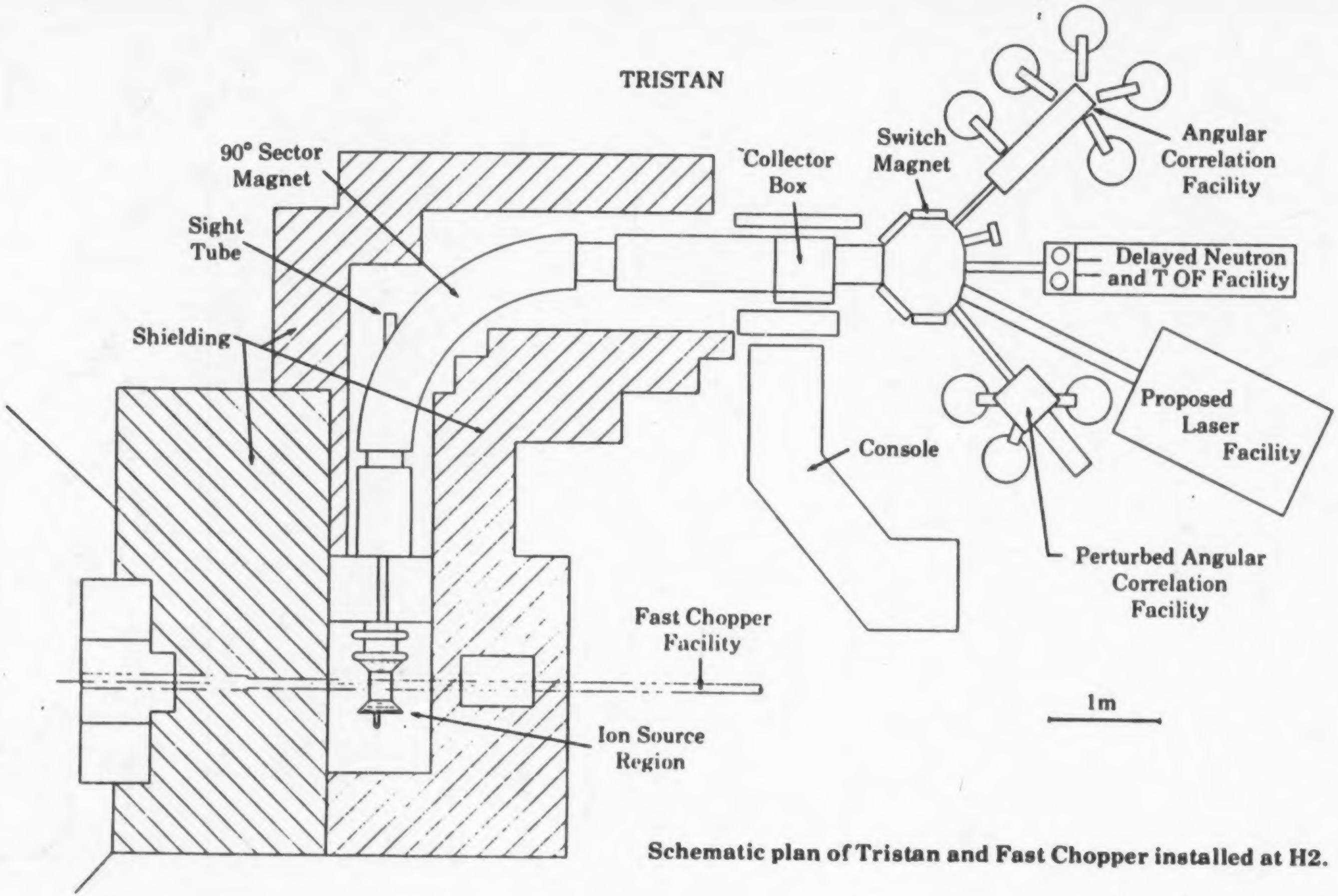
An on-line isotope separator facility called TRISTAN is installed at the H2 beam line. An ion source containing 5g of ^{235}U in a thermal flux of 2.5×10^{10} n/cm^2/sec produces ions of rare short-lived fission products. The ions are electrostatically extracted, accelerated to 50-60 keV, and separated by a 90° bending magnet. At the focal plane of the magnet the ions of the selected mass pass through a slit and are directed by a switching magnet to one of five detector stations. Data are recorded and preprocessed by a CAMAC-linked PDP-11/20 computer system. More detailed analysis is performed using a PDP-11/34 computer which may communicate with the 11/20 via a 300 Mbyte dual port disk. A PDP-11/45 computer is also available and is linked with the 11/34, 11/20, and the H1 11/40 via DMA transfers to a PDP-11/10 which controls a 60 Mbyte data storage disk.

H2 Station Parameters — TRISTAN

Ion Source	Elements Produced	Yield Atoms/sec
Surface Ionization	Rb, Sr, Cs, Ba, Ce, Pr, Nd, Pm	$<10^9$
FEBIAD	Zn, Ga, Ge, As, Se, Br, Kr, Rb, Ag, Cd, In, Sn, Sb, Te, I, Xe, Cs	$<10^7$

Ge(Li), HpGe detectors	γ-ray spectroscopy, γ-γ angular correlations
HpGe,Si(Li) detectors	β spectroscopy, Q_β measurements, conversion electron spectroscopy
25 kG magnet	perturbed angular correlations
^{3}He detectors	delayed neutron spectroscopy, p-n measurements
Time-of-flight spectrometer	low-energy delayed neutron spectroscopy
Dye laser	hyperfine interaction studies

TRISTAN


90° Sector Magnet
Sight Tube
Shielding
`Collector Box
Switch Magnet
Angular Correlation Facility
Delayed Neutron and T OF Facility
Proposed Laser Facility
Console
Perturbed Angular Correlation Facility
Fast Chopper Facility
Ion Source Region
1m

Schematic plan of Tristan and Fast Chopper installed at H2.

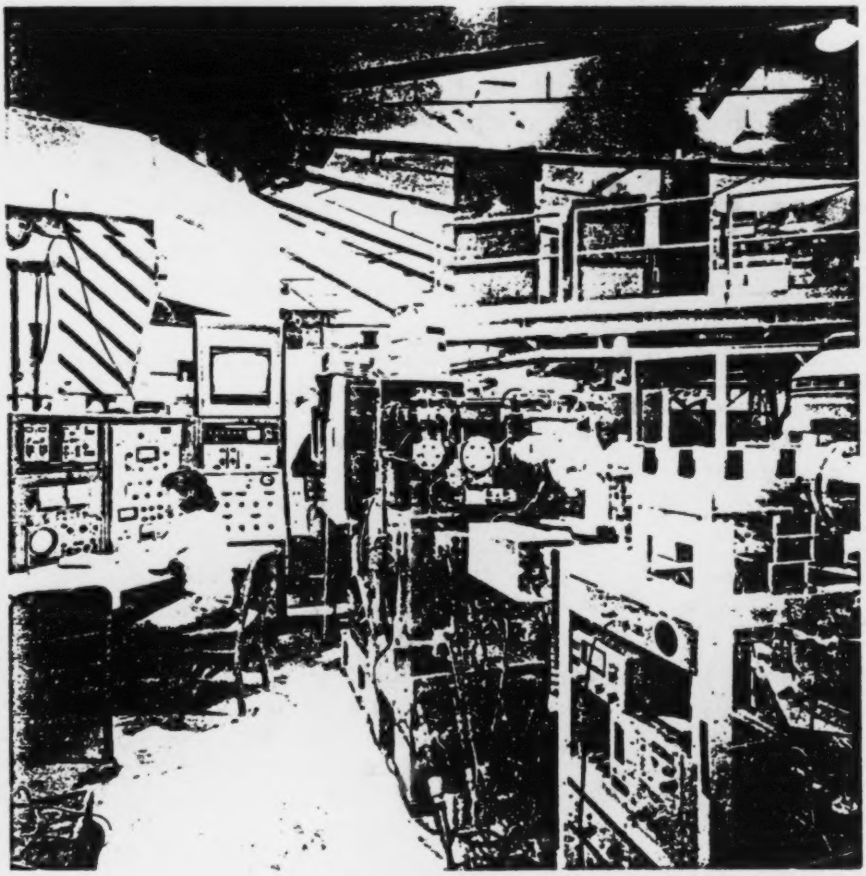
H2 FAST CHOPPER (NUCLEAR PHYSICS)

The H2 beam is also used by a fast chopper facility for time-of-flight analysis of resonance neutron capture γ rays. The need for high intensities requires a high duty cycle and large beam aperture. The correspondingly low neutron resolution limits the device to the energy region below 10 keV for most nuclei. Two rotors are available. Detector stations are placed at flight paths of 22 meters inside the reactor building and at 48 meters in a detector hut outside of the building. The PDP-11/20 based TRISTAN data acquisition system is used to record the γ-ray events following neutron capture. 32 preselected time-of-flight gates sort the pulse-height spectra on-line, eliminating the need for off-line tape scanning.

H2 Station Parameters — Fast Chopper

	Rotor I	Rotor II
Burst Width	5 μsec (minimum)	1 μsec (minimum)
Repetition Rate	1000 cycles/sec	1000 cycles/sec
Band Pass at Full Speed	2 eV to ∞	2 eV to ∞
Flux at 22 meters	$\frac{4.5\times10^4}{E}$ n/cm^2/sec/eV (av.)	$\frac{2.7\times10^3}{E}$ n/cm^2/sec/eV (av.)
Speed Range	1500 to 15000 rpm	1500 to 15000 rpm
Neutron Resolution at 22 meters	$\frac{\Delta E}{E}=0.0067\ E^{1/2}$ (E in eV)	$\frac{\Delta E}{E}=0.003\ E^{1/2}$ (E in eV)
Beam Size	10×7.6 cm^2	10×7.6 cm^2
Neutron Resolution at 48 meters	$\frac{\Delta E}{E}=0.003\ E^{1/2}$ (E in eV)	$\frac{\Delta E}{E}=0.0006\ E^{1/2}$ (E in eV)
Beam Size	20×15 cm^2	20×15 cm^2
Duty Cycle	0.5%	0.1%

Useful energy range: thermal to 10 keV.



TRISTAN Mass Separator Facility located at H2.

H3-A SPECTROMETER FOR PROTEIN CRYSTALLOGRAPHY

This protein crystallographic station features a two-dimensional position-sensitive counter with a four-circle diffractometer. The computer system controls the diffractometer, processes the counter data and permits on-line interactive display. The position-sensitive counter has an efficiency of ~80% with a resolution of 1.5 mm and a counting rate of $\sim 10^5$ c/sec; data are directly encoded into an extended memory. There is a remote controlled monochromator (pyrolytic graphite) with variable circular focusing collimation and provisions for filters.

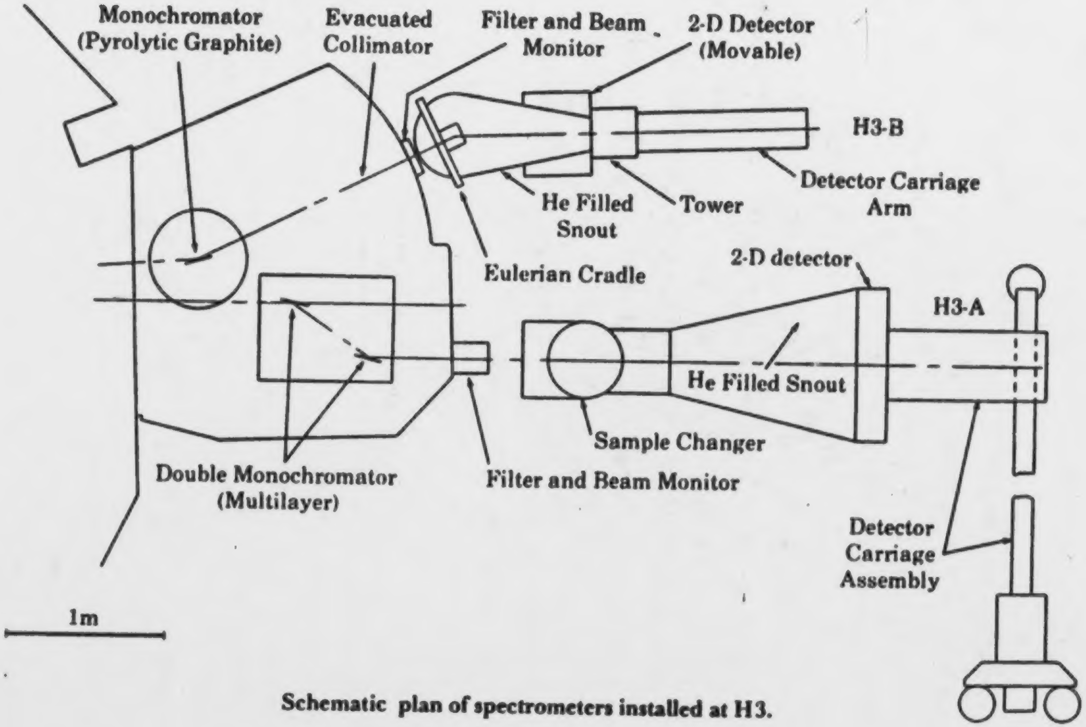
H3-A Station Parameters

Flux at sample	$\sim 2.8\times 10^7$ n/cm^2/sec
Monochromator	(002) pyrolytic graphite, $2\theta=27.15^\circ$ (focusing)
Filter	Pyrolytic graphite
Wavelength λ	1.57 Å (33 meV) (variable)
Beam size at sample (FWHM)	6 mm diameter, 20′ divergence (variable)
Sample scattering angles	$-80^\circ < 2\theta < 80^\circ$
Detector	^{3}He filled position-sensitive detector 20×18 cm, 256×128 pixels. Detector to sample distance is 510 - 2000 mm. Counter resolution= 1.5 mm.
Efficiency	~80%

H3-B INTERMEDIATE RESOLUTION MEMBRANE STATION

The membrane station will feature a two-dimensional position-sensitive detector with a sample changer or exterior cradle. The computer system controls the diffractometer, processes data and permits on-line interactive display. The position-sensitive detector will have an area of ~30 cm×10 cm with a spatial resolution of ~1.5 mm and a maximum rate of $\sim 10^5$ c/sec. Data are directly encoded into an external memory. The double monochromator will use multilayer devices with a wavelength from ~2 Å to 4 Å with an adjustable Δλ.

Completion of the station is expected in the fall of 1984.


Monochromator
(Pyrolytic Graphite)
Evacuated
Collimator
Filter and Beam
Monitor
2-D Detector
(Movable)
H3-B
He Filled
Snout
Tower
Detector Carriage
Arm
Eulerian Cradle
2-D detector
H3-A
He Filled Snout
Sample Changer
Double Monochromator
(Multilayer)
Filter and Beam Monitor
Detector
Carriage
Assembly
1m

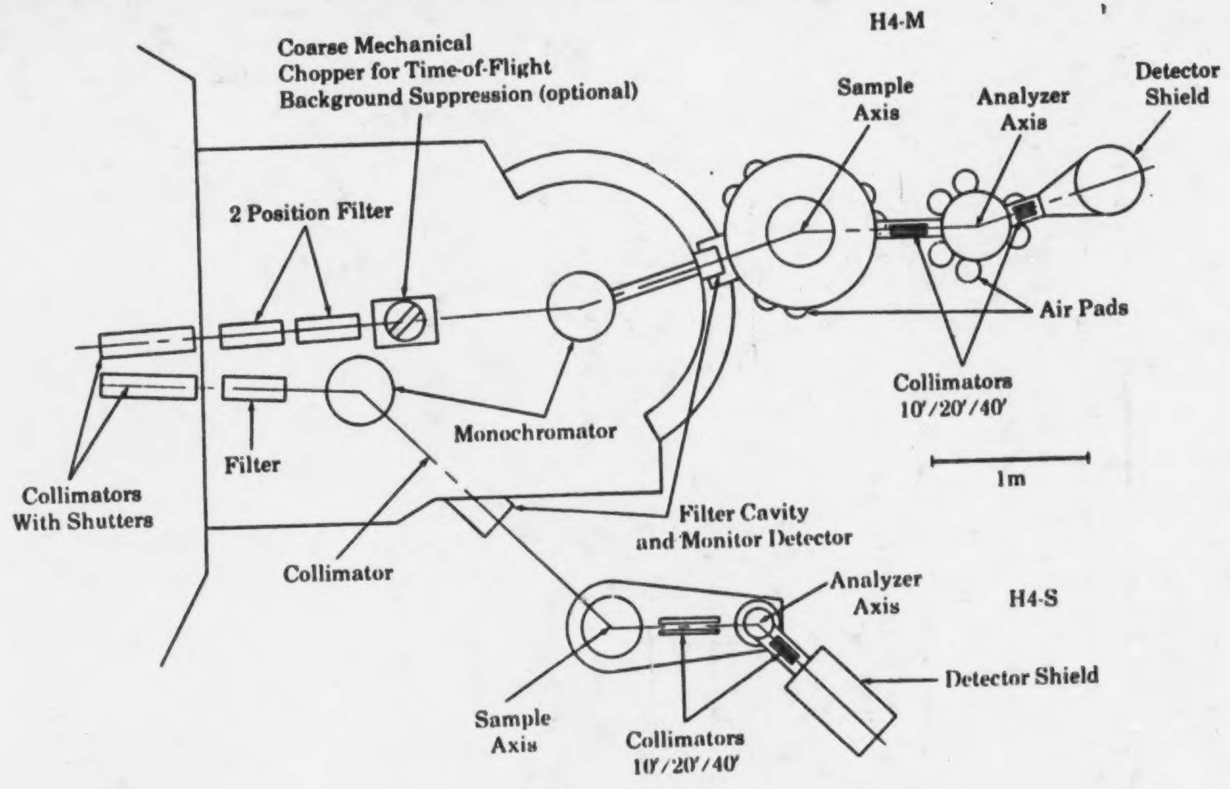
Schematic plan of spectrometers installed at H3.

H4-M SPECTROMETER (POLARIZED BEAM-INELASTIC)

H4-M is currently being developed as a polarized beam spectrometer for elastic and inelastic scattering studies through the US-Japan Cooperative Research Program in Neutron Scattering. Both incident and final neutron energies can be scanned in a conventional triple-axis mode of operation by using either focusing pyrolytic graphite (002) or Heusler (111) polarizing monochromators or analyzers. The sample table is equipped with the standard two arm goniometer which is compatible with a variety of cryostats and furnaces. Sample and analyzer tables move on air pads, and the distances between monochromator, sample, and analyzer are adjustable. For polarized beam work, high efficiency flat coil π-flippers and guide fields are available. Time-of-flight capabilities with several detectors will also be implemented.

H4-M Station Parameters

Flux at monochromator position	3.5×10^9 n/cm^2-sec
Monochromator scattering angle	$10^\circ<2\theta_M<108^\circ$
E_0 or λ_0 (PG 002)	$2.8<E_0<240$ meV $5.43>\lambda_0<0.58$ Å
Beam size	3.8×7.6 cm^2
Sample scattering angle	$-20^\circ<2\theta_S<155^\circ$
Drum to sample axis distance	$0.7<L<3$ m
Detector	^{3}He
In-pile collimation	20′, 40′
External collimation	10′, 20′ or 40′


H4-M
Coarse Mechanical
Chopper for Time-of-Flight
Background Suppression (optional)
Sample
Axis
Analyzer
Axis
Detector
Shield
2 Position Filter
Air Pads
Collimators
10′/20′/40′
Monochromator
Filter
Collimators
With Shutters
1m
Filter Cavity
and Monitor Detector
Collimator
Analyzer
Axis
H4-S
Detector Shield
Sample
Axis
Collimators
10′/20′/40′

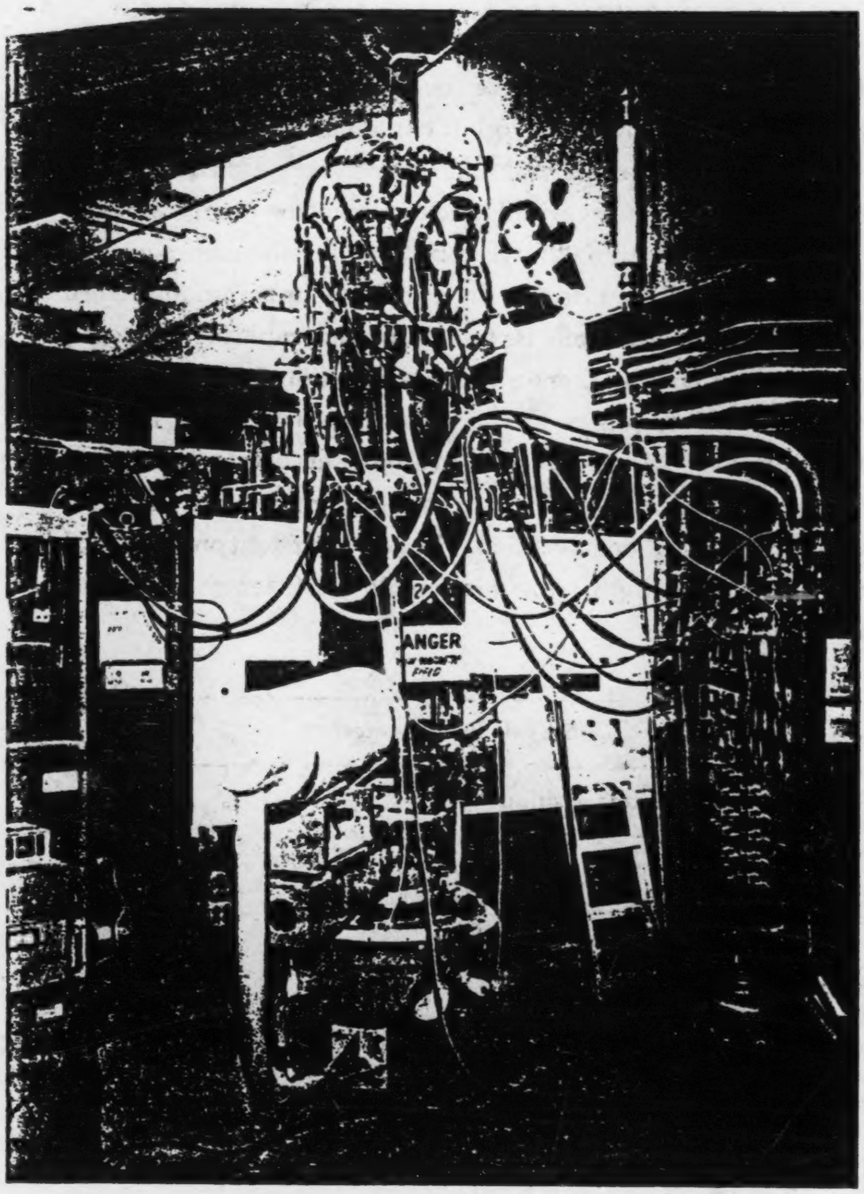
Schematic of neutron spectrometers installed at H4.

H4-S SPECTROMETER (DIFFRACTION AND SMALL ANGLE SCATTERING)

H4-S provides a double-axis spectrometer for diffraction and also accommodates small angle scattering studies for molecular biology featuring a 2D position-sensitive detector. A fixed monochromator takeoff angle of $2\theta_M=41.1^\circ$ gives an incident energy of $E_0=14.8$ meV, from pyrolytic graphite; other energies are available by changing to different monochromators. A standard goniometer accommodates a wide range of cryostats, furnaces, or magnets.

H4-S Station Parameters

Flux at monochromator position	4.0×10^9 n/cm^2-sec
Monochromator scattering angle	$2\theta_M=41.1^\circ$
E_0 or λ_0 (PG 002)	14.8 meV (2.36 Å)
Beam size at sample	5 (h)×2.5 (w) cm^2 or 6 mm diam
Sample scattering angle	$-30^\circ<2\theta_S<125^\circ$
In-pile collimation	20′, 40′
External collimation	10′, 20′, 40′
Detector	BF_3 and ^{3}He (2D), 17×17cm^2



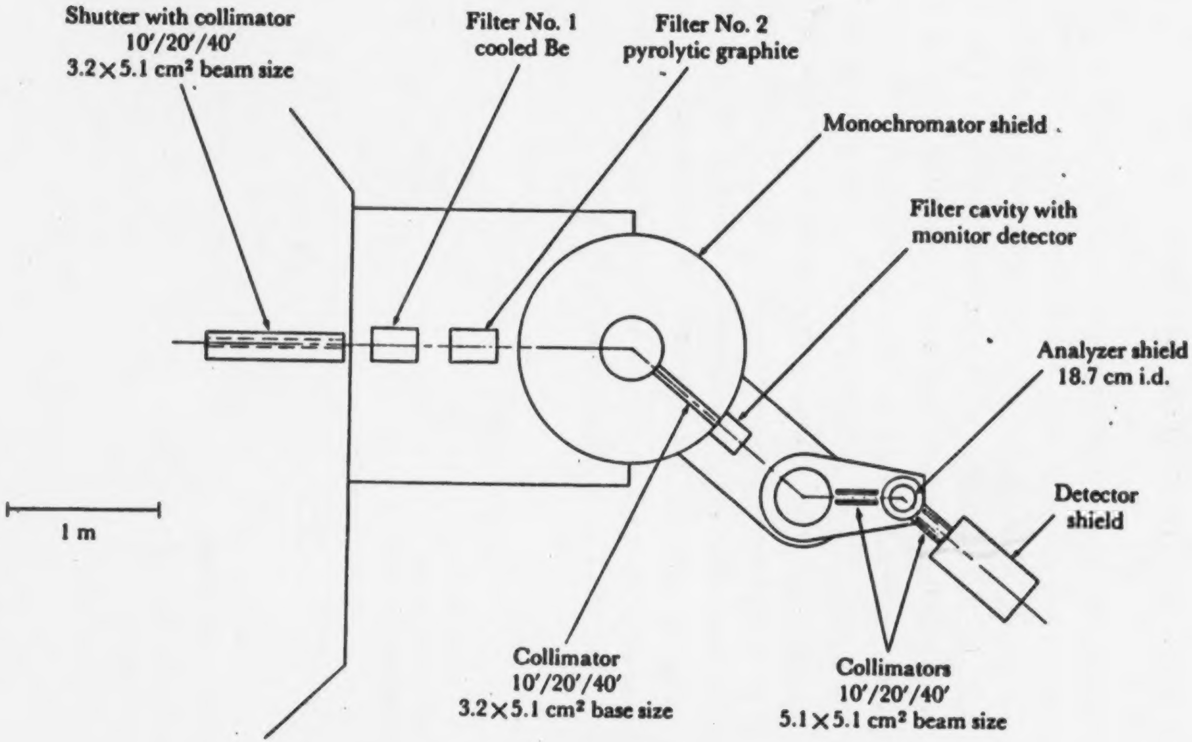
H4-S Spectrometer with a dilution refrigerator on sample axis.

H5 SPECTROMETER (INELASTIC SCATTERING)

H5 is a triple-axis spectrometer used primarily for single crystal inelastic experiments, although it can often be used effectively for studying polycrystalline and amorphous samples. The instrument is fully automated for variable incident neutron energies. It is normally equipped with (002) pyrolytic graphite monochromator and analyzer crystals, but Be, Cu, Zn, and Ge monochromators are also available. Optional in-pile Be and pyrolytic graphite filters are provided for removing higher order contamination. The sample table is equipped with manual two-axis goniometers with a ±10° range, and is compatible with a variety of available cryostats and furnaces. External collimation (other than in-pile) is provided by Soller slits with a 5.1×5.1 cm^2 cross section. The beam incident on the sample is monitored by a high transmission, low efficiency uranium foil detector.

H5 Station Parameters

Flux at monochromator position (20′ in-pile collimation)	4.2×10^9 n/cm^2-sec
Monochromator scattering angle	$10^\circ<2\theta_M<55^\circ$
E_0 or λ_0 (PG 002)	$8.5<E_0<240$ meV $3.09>\lambda_0>0.58$ Å
Beam size	5×3.1 cm^2
Sample scattering angle	$-45^\circ<2\theta_S<125^\circ$
Analyzer scattering angle	$-100^\circ<2\theta_A<100^\circ$
In-pile collimation	10′, 20′, or 40′
External collimation	10′, 20′, or 40′
Detector	BF_3


Shutter with collimator
10′/20′/40′
3.2×5.1 cm² beam size
Filter No. 1
cooled Be
Filter No. 2
pyrolytic graphite
Monochromator shield
Filter cavity with
monitor detector
Analyzer shield
18.7 cm i.d.
Detector
shield
1 m
Collimator
10′/20′/40′
3.2×5.1 cm² base size
Collimators
10′/20′/40′
5.1×5.1 cm² beam size

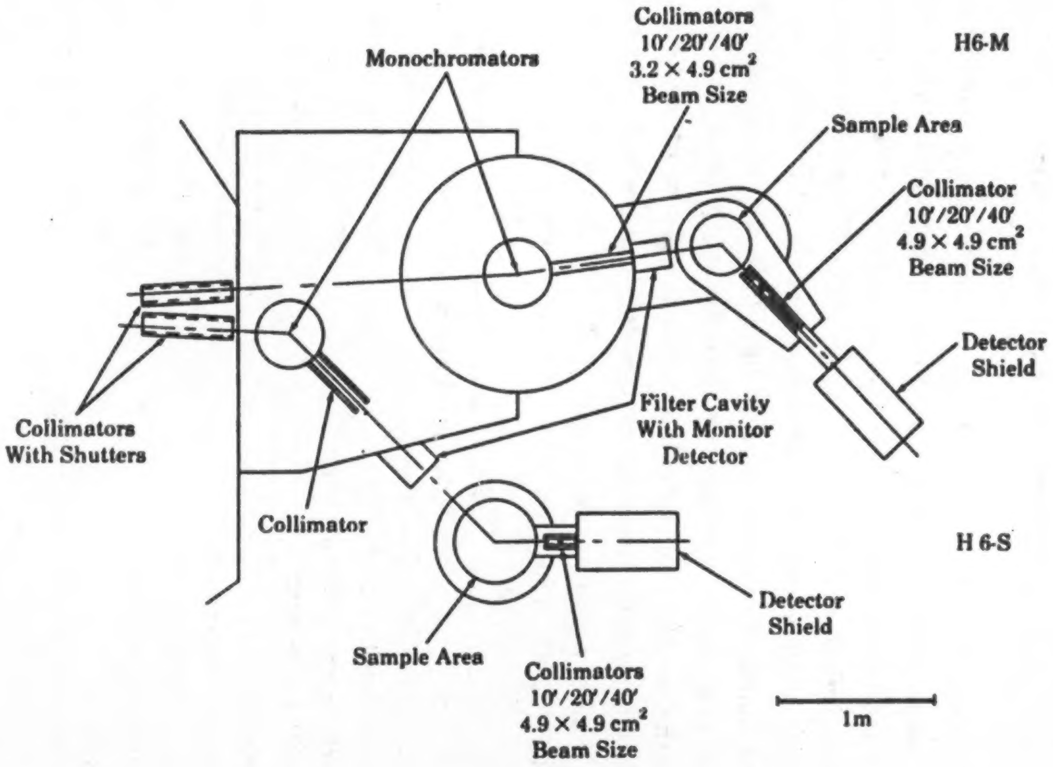
Schematic plan of triple-axis spectrometer installed at H5.

H6-M SPECTROMETER (DIFFRACTION)

H6-M is a triple-axis spectrometer used primarily for single crystal elastic studies. A single crystal monochromator is used with a variable scattering angle allowing for a choice of incident wavelengths. The spectrometer is equipped with a computer-controlled 4-circle goniometer which allows complete freedom in orienting single crystal samples. The instrument has an analyzer arm which will permit inelastic measurements, or permit diffraction measurements for zero energy transfer, thus reducing background. An extensive library of operating programs provides automatic crystal centering, unit-cell and orientation-matrix refinements, and collection of diffraction intensities by the step-scan method. Raw step-scan profiles are output on magnetic tape and processed off-line in the BNL CDC-CYBER 70/76 or VAX 11/780 computing system.

H6-M Station Parameters

Flux at monochromator (20′ in-pile collimation)	4.1×10^9 n/cm^2-sec
Monochromator scattering angle	$21^\circ < 2\theta_M < 56^\circ$
λ_0 or E_0 (Be 002)	$1.69 > \lambda_0 > 0.65$ Å $28.5 < E_0 < 192$ meV
Beam size (maximum)	3.2 (h)×4.9 (w) cm^2
Sample scattering angle	$-30^\circ < 2\theta_S < 113^\circ$
Analyzer scattering angle	$-120^\circ < 2\theta_A < 120^\circ$
In-pile collimation	1.9 cm diam hole, or 20′
External collimation	10′, 20′, or 40′
Detector	BF_3


H6-M
Monochromators
Collimators
10′/20′/40′
3.2 × 4.9 cm²
Beam Size
Sample Area
Collimator
10′/20′/40′
4.9 × 4.9 cm²
Beam Size
Detector
Shield
Collimators
With Shutters
Filter Cavity
With Monitor
Detector
Collimator
H 6-S
Detector
Shield
Sample Area
Collimators
10′/20′/40′
4.9 × 4.9 cm²
Beam Size
1m

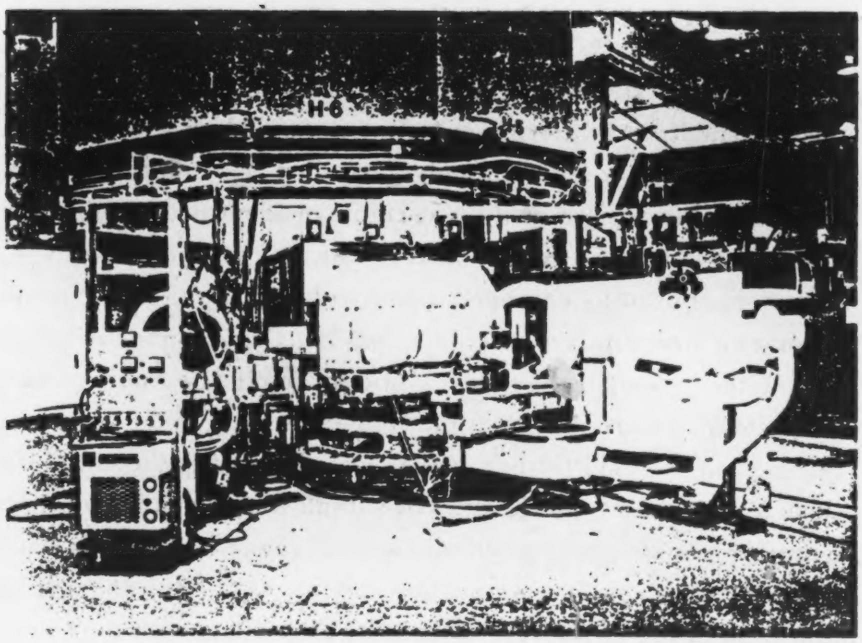
Schematic plan of spectrometers installed at H6.

H6-S SPECTROMETER (DIFFRACTION)

H6-S is a spectrometer used primarily for single crystal elastic scattering measurements. A single crystal monochromator is used with a fixed scattering angle ($2\theta_M=34°$) corresponding to $\lambda=1.16$ Å for the Ge (220) reflection or $\lambda=1.05$ Å for Be (002). The spectrometer is equipped with a computer-controlled 4-circle goniometer which allows complete freedom in orienting single crystal samples. An extensive library of operating programs is available for automatic centering, unit cell and orientation matrix refinement, and collection of diffraction intensities by the step-scan method. Raw step-scan profiles are output on magnetic tape and processed off-line on the BNL CDC-CYBER 70/76 or VAX 11/780 computing system.

H6-S Station Parameters

Flux at monochromator	6.6×10^9 n/cm^2-sec
Monochromator scattering angle	$2\theta_M=34°$
λ, Ge (220) or Be (002)	1.16 Å or 1.05 Å
Beam size	0.6 cm — 2.5 cm (diam)
Sample scattering angle	$-21°<2\theta_S<109°$
In-pile collimation	20′, 40′
External collimation	10′, 20′, or 40′
Detector	BF_3



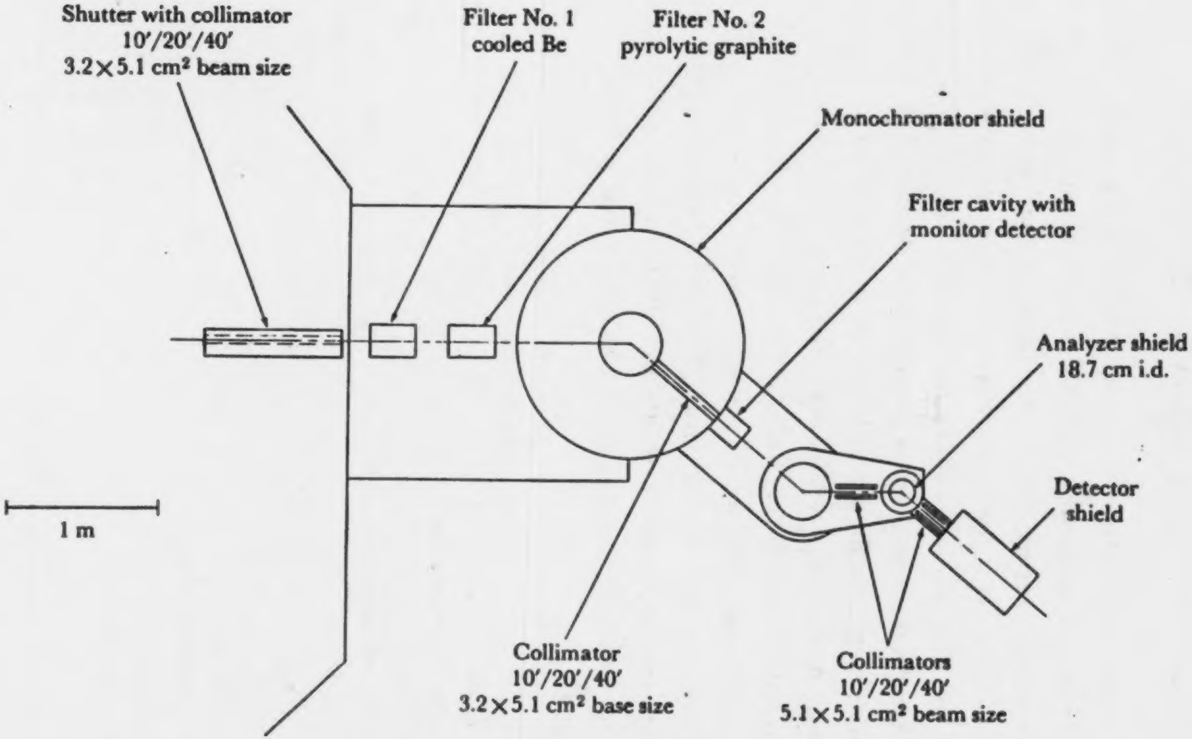
H6 Experimental Station.

H7 SPECTROMETER (INELASTIC SCATTERING)

H7 is a triple-axis spectrometer used primarily for single crystal inelastic neutron scattering experiments, although it can also be used effectively for studying polycrystalline and amorphous samples. H7 is fully automated for variable incident neutron energies and scans with a fixed final energy can be performed. The spectrometer is normally equipped with pyrolytic graphite (002) monochromator and analyzer crystals, but Be, Cu, Zn, and Ge monochromators are also available. Optional in-pile Be and pyrolytic graphite filters are provided for removing higher order beam contamination. Be and PG filters can also be placed after the sample for the fixed analyzer type of scan. The sample table is equipped with a manual two-axis goniometer with a $\pm 10^\circ$ range and is compatible with a variety of available cryostats and furnaces. External collimation (other than in-pile) is provided by Soller slits with a 5×5 cm^2 cross section.

H7 Station Parameters

Flux at monochromator position (20′ collimation in-pile)	4.1×10^9 n/cm^2-sec
Monochromator scattering angle	$10^\circ<2\theta_M<75^\circ$
E_0 or λ_0 (PG 002)	$4.9<E_0<240$ meV $4.1>\lambda_0>0.58$ Å
Beam size at sample	5 (h)$\times$3.1 (w) cm^2
Sample scattering angle	$-45^\circ<2\theta_S<128^\circ$
Analyzer scattering angle	$-100^\circ<2\theta_A<100^\circ$
In-pile collimation	10′, 20′, 40′
External collimation	10′, 20′, 40′
Detector	BF_3


Shutter with collimator
10′/20′/40′
3.2×5.1 cm² beam size
Filter No. 1
cooled Be
Filter No. 2
pyrolytic graphite
Monochromator shield
Filter cavity with
monitor detector
Analyzer shield
18.7 cm i.d.
Detector
shield
1 m
Collimator
10′/20′/40′
3.2×5.1 cm² base size
Collimators
10′/20′/40′
5.1×5.1 cm² beam size

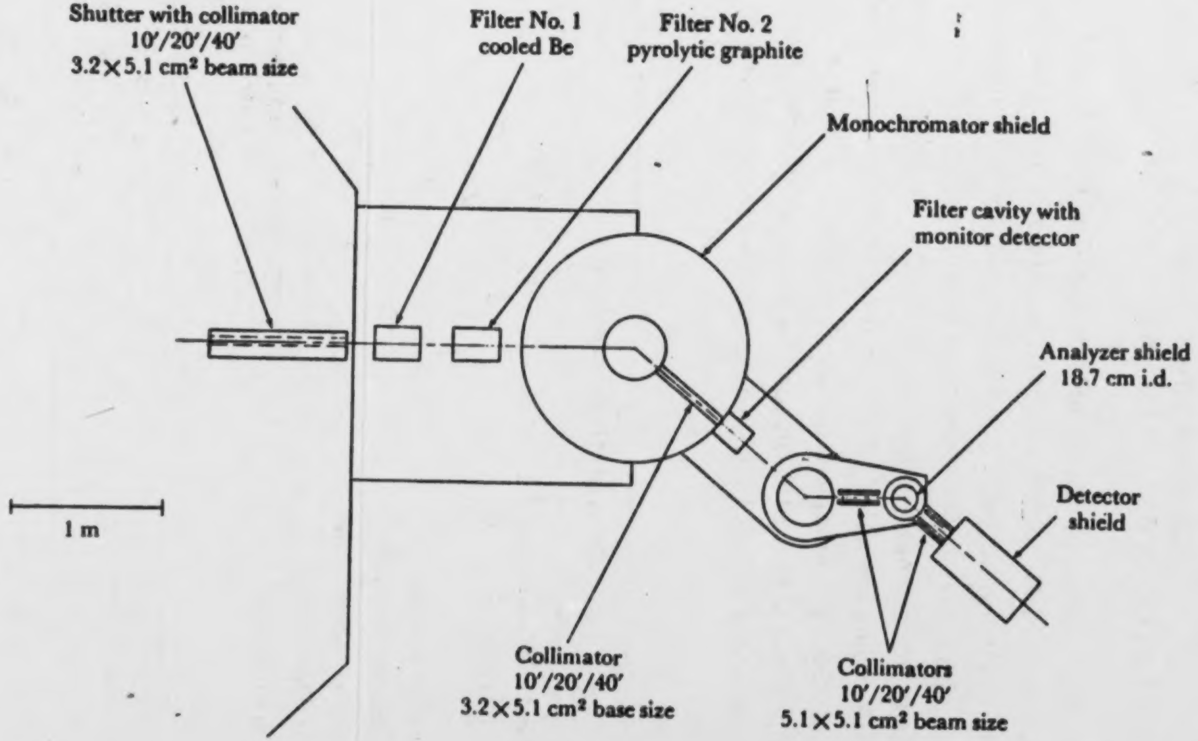
Schematic plan of triple-axis spectrometer installed at H7.

H8 SPECTROMETER (POLARIZED BEAM, INELASTIC SCATTERING)

H8 is a triple axis spectrometer used primarily for single crystal inelastic neutron scattering experiments. It is equipped with a monochromator housing that can accommodate either a PG (002) or a Heusler (111) crystal, for unpolarized and polarized neutron work, respectively. The incident energy can be varied remotely so scans with a fixed final energy can be performed. A Heusler (111) analyzing crystal, magnetic flippers, and guide fields can easily be positioned to allow for use as a fully polarized beam instrument. Cooled Be and pyrolytic graphite crystals are available for removing higher order beam contamination. The sample table is equipped with a manual two-axis goniometer with a ±10° range and is compatible with a variety of available cryostats and furnaces. External collimation is provided by Soller slits with a 5×5 cm^2 cross section.

H8 Station Parameters

Flux at monochromator position (20′ in-pile collimation)	4.2×10^9 n/cm^2-sec
Monochromator scattering angle	$10^\circ<2\theta_M<75^\circ$
E_0 or λ_0 (PG 002)	$4.9<E_0<240$ meV $4.1>\lambda_0>0.58$ Å
Beam size	5 (h)×3.1 (w) cm^2
Sample scattering angle	$-45^\circ<2\theta_S<140^\circ$
Analyzer scattering angle	$-100^\circ<2\theta_A<100^\circ$
In-pile collimation	10′, 20′, 40′
External collimation	10′, 20′, 40′
Detector	BF_3


Shutter with collimator
10′/20′/40′
3.2×5.1 cm² beam size
Filter No. 1
cooled Be
Filter No. 2
pyrolytic graphite
Monochromator shield
Filter cavity with
monitor detector
Analyzer shield
18.7 cm i.d.
Detector
shield
1 m
Collimator
10′/20′/40′
3.2×5.1 cm² base size
Collimators
10′/20′/40′
5.1×5.1 cm² beam size

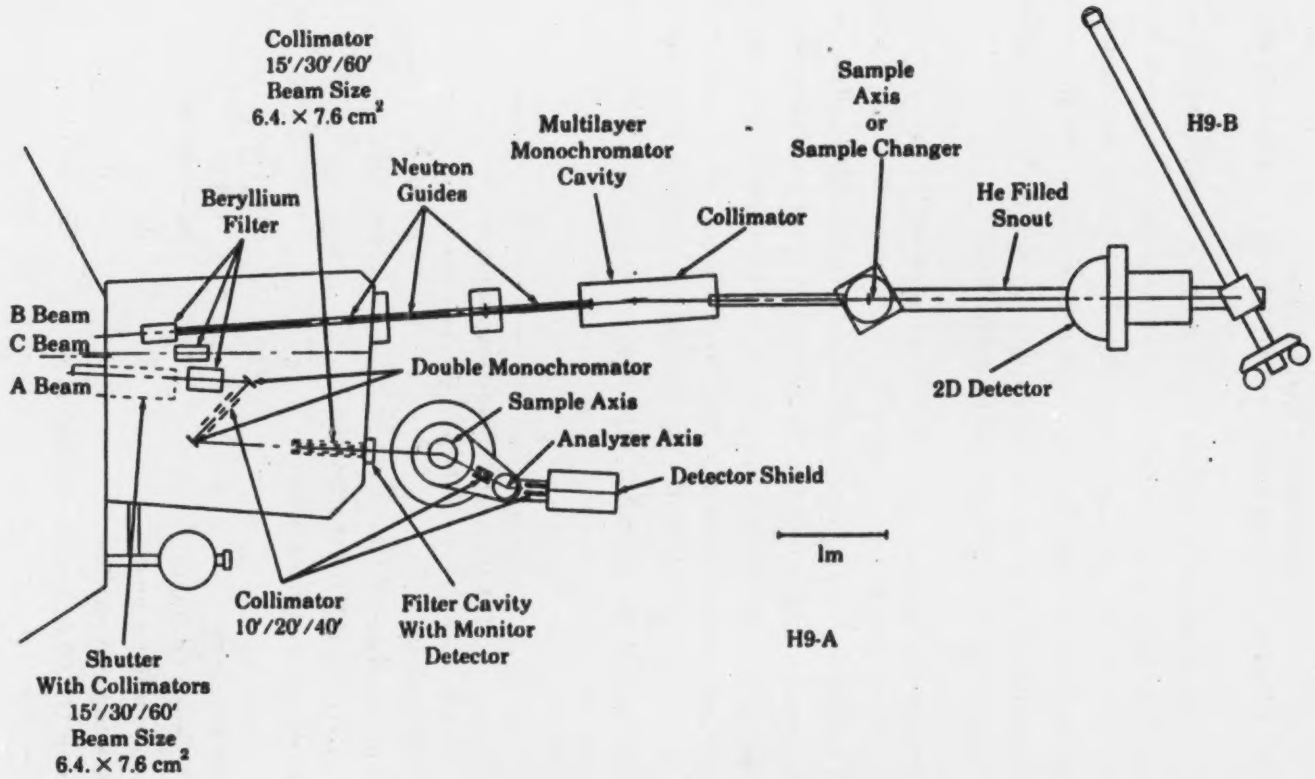
Schematic plan of triple-axis spectrometer installed at H8.

H9-A SPECTROMETER (INELASTIC SCATTERING – COLD NEUTRONS)

H9-A is a triple-axis type spectrometer situated on the cold neutron facility. It is used for high resolution inelastic neutron scattering studies of single crystal, polycrystalline, or amorphous samples. It is equipped with a double monochromator arrangement which allows for large monochromator scattering angles. A Be filter is placed before the monochromator for elimination of higher order beam contamination. The sample table is equipped with a manual two-axis goniometer with a ±10° tilt range about two orthogonal horizontal axes, and is compatible with a range of available cryostats and furnaces.

H9-A Station Parameters

Monochromator scattering angle	$41^\circ < 2\theta_M < 134^\circ$
E_0 or λ_0 (PG 002)	$2.15 < E_0 < 14.7$ meV $6.2 > \lambda_0 > 2.35$ Å
Beam size at sample	7.5 (h)×5 (w) cm^2
Sample scattering angle	$-50^\circ < 2\theta_S < 150^\circ$
Analyzer scattering angle	$-125^\circ < 2\theta_A < 125^\circ$
In-pile collimation	15′, 30′, or 60′
External collimation	15′, 30′, or 60′ before sample 10′, 20′, or 40′ after sample
Detector	BF_3


Collimator
15′/30′/60′
Beam Size
6.4. × 7.6 cm²
Multilayer
Monochromator
Cavity
Sample
Axis
or
Sample Changer
H9-B
Neutron
Guides
Beryllium
Filter
He Filled
Snout
Collimator
B Beam
C Beam
A Beam
Double Monochromator
Sample Axis
Analyzer Axis
Detector Shield
2D Detector
lm
Collimator
10′/20′/40′
Filter Cavity
With Monitor
Detector
H9-A
Shutter
With Collimators
15′/30′/60′
Beam Size
6.4. × 7.6 cm²

Schematic plan of spectrometers installed at H9.

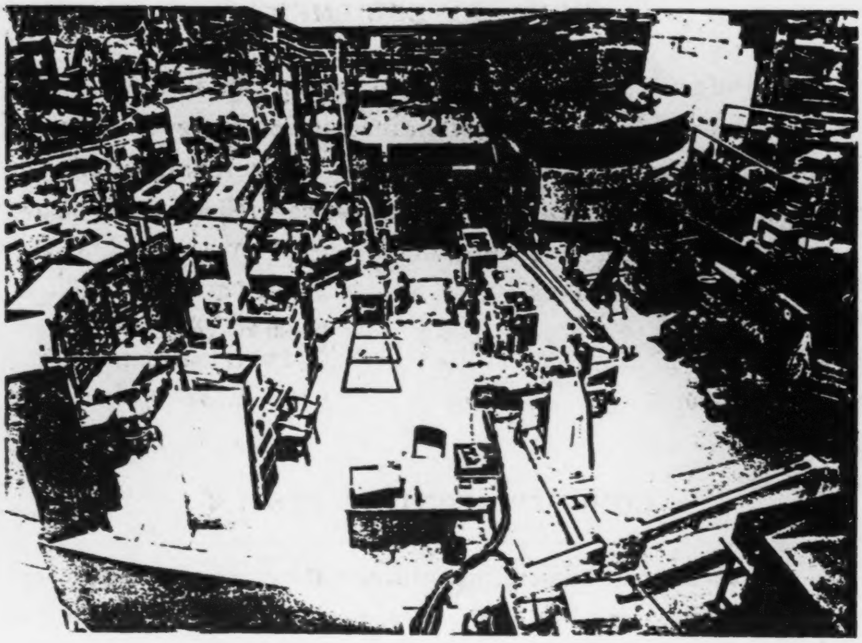
H9-B SPECTROMETER
(SMALL ANGLE SCATTERING – BIOLOGICAL STRUCTURE)

The H9-B spectrometer is used for small angle diffraction studies on macromolecular biological structures. Samples can be oriented on a vertical axis or by an automated sample changer, and a two-dimensional detector can be positioned automatically on an arc of variable radius. This allows for the required flexibility to investigate both solution samples and oriented preparations.

The spectrometer utilizes a Be-filtered cold moderator beam emerging from Ni-coated neutron guides (25.4×50.8 mm). Monochromatization is achieved with exchangeable Fe-Mn or Ge-Mn multilayers with bilayer spacings between 50 and 150 Å. The monochromatic beam is collimated over a length of 2 m by a series of apertures of decreasing diameter. Typically, the primary beam has a diameter of 6 mm at the sample. A PDP 11-34 computer with a large external memory is used for experimental control and preliminary data analysis.

H9-B Spectrometer Parameters

Wavelength range	4 — 10 Å
Wavelength spread (FWHM)	6 — 15%
Beam divergence (FWHM, horizontal)	14′
Flux at sample (5 Å, 6 mm beam)	1 — 2×10^6 n/cm^2-sec
Detector area	50×50 cm^2
Detector resolution	3 mm
Sample-detector distance	50 — 200 cm
Range of scattering angles	0 — 45°
Best spectrometer resolution	1000 Å
Minimum Q (λ=5 Å, 2 m detector distance)	0.002 Å^{-1}



H9 Experimental Station.

ANCILLARY EQUIPMENT

A variety of cryostats, furnaces, and magnets is available to control the sample environment. Most of the instruments have standardized mounts or adaptors so as to permit ready interchangeability at various experimental stations. The ranges covered are given below.

Cryostats and refrigerators	0.03K<T<325K
Furnaces and ovens	300K<T<1700K
Magnets	0—90 kG vertical 0—24 kG horizontal
Pressure	0 to 30 k bar

COMPUTER CONTROL SYSTEM

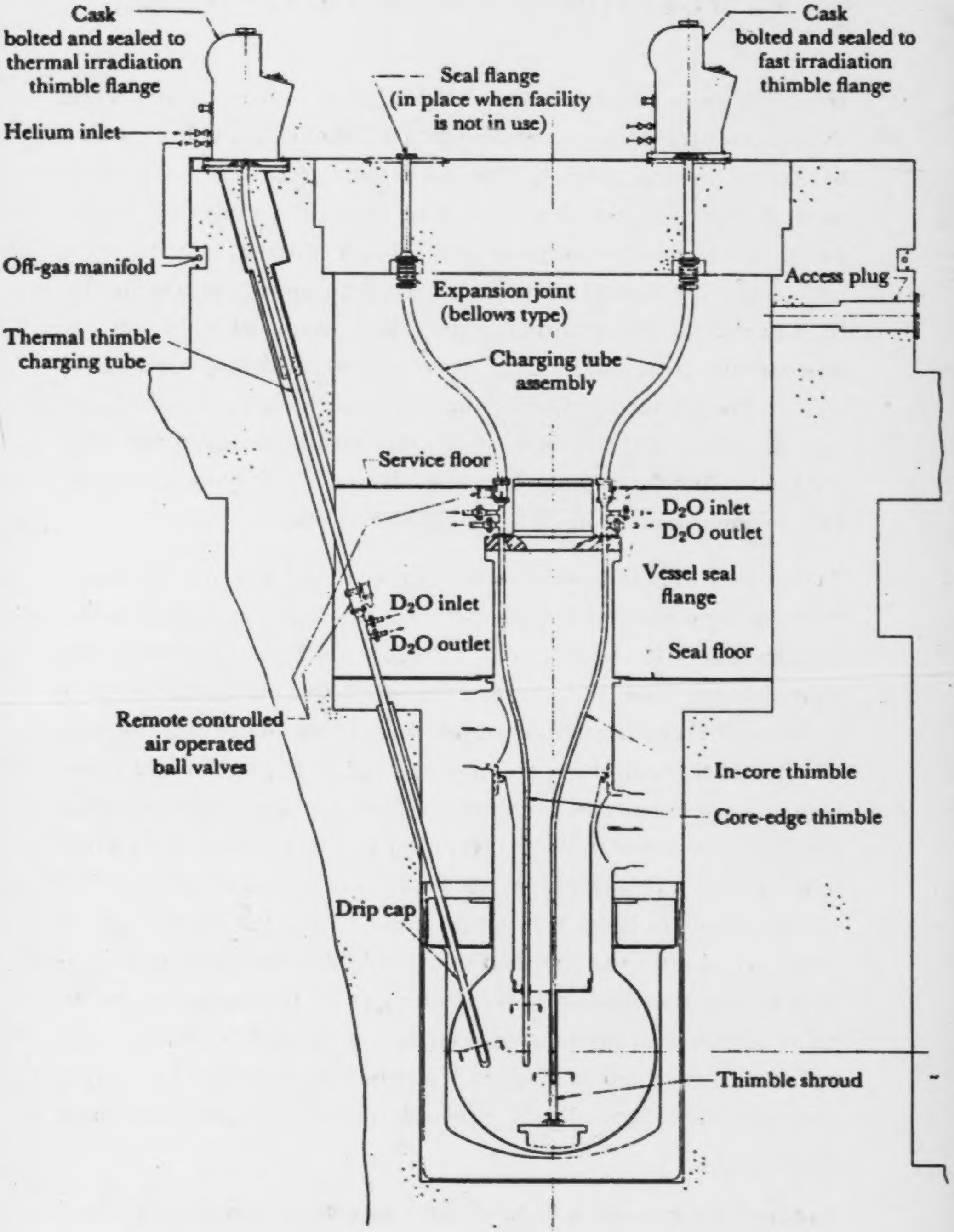
The various scientific disciplines utilizing the reactor have different needs for control and data acquisition. Each instrument is computer controlled and data are collected and stored either on magnetic tape or on disc. Some preliminary on-line data analysis is performed at the HFBR but many of the data are transferred to a larger computer at the user's laboratory where the final data analyses are performed.

V. Irradiation of Samples at the HFBR

Irradiation experiments at the HFBR play an important role in the overall research program. Seven vertical thimbles provide a variety of neutron energy spectra for sample irradiations. Thermal or slow neutrons are used primarily for neutron activation analysis ("fingerprinting" unknown substances by artificially induced radioactivity) and for the production of special purpose radioisotopes. Due to the high neutron flux available, it is possible to produce highly radioactive samples from small quantities of material (high specific activity), and to produce certain isotopes in quantities unattainable by any other practical means. Fast neutron irradiations are vital to the study of radiation damage in materials and are playing an important role in the program to develop a fusion reactor.

Three of the irradiation thimbles (V10, V11, and V12) are located in the reflector portion of the reactor, while the others are positioned at the core edge (V13 and V14) and at the core center (V15 and V16). The thimbles are fitted with a set of reentrant tubes connected to a separate D_2O cooling system which circulates a flow of 45 liters/min downward through the center and upward through the outer annular region of each tube. Samples are placed in aluminum capsules which are immersed in the D_2O for cooling. Each capsule is attached to the end of a 10 meter length of 6 mm diameter aluminum tubing which is used to lower the sample capsule into the reactor and to withdraw it after the irradiation. In addition, this tubing can be used to vent the capsule, to fill it with gas for heat transfer, and to bring out a pair of thermocouple leads, if desired. A hydraulic "rabbit" is also available at Facility V11 which permits rapid insertion and retrieval of samples for precisely-timed irradiations of short duration.

Irradiations can be scheduled by contacting Reactor Research Coordination at extension 4056 or 4436. All proposed irradiations


Cask
bolted and sealed to
thermal irradiation
thimble flange
Helium inlet
Seal flange
(in place when facility
is not in use)
Cask
bolted and sealed to
fast irradiation
thimble flange
Off-gas manifold
Expansion joint
(bellows type)
Access plug
Thermal thimble
charging tube
Charging tube
assembly
Service floor
D_2O inlet
D_2O outlet
Vessel seal
flange
D_2O inlet
D_2O outlet
Seal floor
Remote controlled
air operated
ball valves
In-core thimble
Core-edge thimble
Drip cap
Thimble shroud

Elevation showing location of several irradiation thimbles within the reactor.

are reviewed by the Research Coordinator for their potential impact on reactor safety. Proposed irradiations of samples which might cause large reactivity changes or present unusual hazards, such as those involving fissionable materials, or materials which can decompose and react with vessel components or reactor coolant, must be reviewed and approved by the Reactor and Critical Experiments Safety Committee before they can be placed in the reactor.

HFBR Irradiation Facilities

Facility	Flux, neutrons/cm^2-sec Thermal	Flux, neutrons/cm^2-sec Fast (>1 MeV)	Heating Rate, W/g (in aluminum)	Useable Dimensions Diam (cm)	Useable Dimensions Length (cm)
V10	2.7×10^{14}	7.5×10^{11}	0.38	2.4	7.6
V11	1.5×10^{14}	9.0×10^{10}	0.23	2.0	7.6
V12	3.8×10^{14}	8.3×10^{11}	1.20	2.4	7.6
V13*	8.3×10^{14}	9.0×10^{13}	6.0	1.5	7.6
V14	8.3×10^{14}	9.0×10^{13}	6.0	1.9	7.6
V15	2.0×10^{14}	3.0×10^{14}	12.0	1.9	7.6
V16*	2.0×10^{14}	3.0×10^{14}	12.0	1.5	7.6

*Accessible for placement and removal of samples only during reactor shutdown. V13 and V16 can accommodate two samples each of the size given.

3.2 National Synchrotron Light Source (NSLS)

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

Answer:

A. VUV Storage Ring

Soft X-rays are being used by IBM to replicate sub-micron integrated circuit features onto photoresist material. A research team from the State University of New York at Stony Brook has developed a soft X-ray microscope capable of looking at the internal structure of cells in aqueous solutions with sub-micron resolution. Soft X-ray holography is also being performed on this storage ring. Photoemission spectroscopy is being utilized to look at the electronic band structures of semiconductor and metal surfaces and to study photoionization processes in gases. There is considerable interest in the exciting energy region up to and above the carbon K-edge (photon energy = 285 eV). High resolution (0.1 eV) ESCA (electron spectroscopy for chemical analysis) studies will be performed to determine differences in core level shifts between bulk atoms and atoms on surfaces with steps and/or chemisorbed species. This information can be useful in explaining catalytic processes. The high intensity of synchrotron radiation is essential in gas phase spectroscopy studies where excitation and photoionization processes of low density (10^{13} cm^{-3}) atom and molecular samples are studied. VUV circular dichroism results are being used to confirm biological structures obtained from X-ray diffraction.

B. X-Ray Storage Ring

The high intensity and brightness of X-ray radiation from the NSLS 2.5 GeV storage ring will make possible measurements on micron-sized samples and allow experimenters to study dynamical effects in different systems. Experimenters will obtain X-ray diffraction data from crystals less than 20 microns in diameter, including a number of technologically-important crystals such as zeolites. X-ray diffraction will be used to study structural effects and phase transitions induced by external perturbations such as laser irradiation, temperature changes, stress, etc. Powder diffraction data will be obtained on more complicated structures than could be previously examined with conventional X-ray sources. X-ray topography will be used to study defects over large sample volumes and to study dynamical effects such as plastic deformation, fracture, precipitation and melting. A number of X-ray techniques will be employed to study surface structures. These include X-ray scattering, surface crystallography, EXAFS (extended X-ray absorption fine structure), SEXAFS (surface EXAFS), NEXAFS (near edge EXAFS), and photoelectron diffraction. An X-ray microprobe will detect impurity levels on the parts per billion scale for sample areas of several microns. Small angle scattering measurements will be conducted to look at long range order in metal alloys and polymers and to examine biological molecules. Inelastic X-ray scattering will be used to study dynamical excitation on the 1 to 100 meV level.

Monochromatic, polarized gamma rays ($E < 500$ MeV), produced by the backscattering of laser beams by 2.5 GeV electrons, will be used for nuclear physics experiments. High-contrast pictures of blood vessels in animal hearts will be obtained using an angiography technique. The NSLS has plans for utilizing this low-risk technique on human patients in the future.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

Answer: The NSLS has the world's highest brightness continuous sources of X-ray and UV radiation. It is the first X-ray facility in the U.S. dedicated for use as a synchrotron light source. The combination of a 2.5 GeV electron storage ring for X-ray research and a 750 MeV electron storage ring for UV research will allow scientists to perform complementary X-ray and UV measurements on their samples. The NSLS has a very large capacity - there will be approximately 90 X-ray and UV beam lines running simultaneously at full capacity. This represents a low operational cost per beam line as reflected by the full cost recovery fee of $40/hour that proprietary users will be charged in FY 1984.

The original Green-Chasman lattice design provided insertion straights for special undulators and wiggler devices which will further enhance the photon brightness and/or intensity. A Phase II expansion is underway for implementing state-of-the-art undulator and wiggler devices and beam lines.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

Answer: In the materials science/solid state physics area there are experimental facilities for performing X-ray scattering, EXAFS, NEXAFS, crystallography, energy dispersive diffraction, topography, X-ray photoelectron spectroscopy, X-ray microprobe, X-ray interferometry, angle-resolved UV photoemission spectroscopy, SEXAFS, lithography and holography. These facilities include special high resolution crystal and grating monochromators, six circle spectrometers, high temperature/high pressure cells, and UHV sample chambers. In the chemical sciences there are experimental facilities for chemical crystallography/diffuse scattering and for photochemistry. The crystallography beam line will have capabilities of measuring very small crystals such as zeolites. The photochemistry facilities include a windowless supersonic nozzle beam apparatus and a fast photon counting system for fluorescence lifetime studies. In the area of medical research there will be facilities for performing angiography studies. There will be a nuclear physics beam line for conducting experiments with polarized γ-rays with energies up to 500 MeV.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer: Experimental operations began on the UV ring in August, 1982. There are now a large number of beam lines producing new results in diverse scientific areas. A few of these results are highlighted below.

The high intensity and collimation of synchrotron radiation from the VUV storage ring has been utilized on the IBM lithography line (Port U6) to expose a number of photoresists. Features as small as 0.25 microns have already been replicated successfully with high aspect ratios. The large increase in intensity of the storage ring over conventional X-ray sources should allow much greater throughput with simple resist processing. If the economic feasibility of using synchrotron radiation for X-ray lithography is demonstrated at the NSLS, there could be a greatly expanded use of synchrotron radiation in the U.S. with storage rings becoming an integral part of semiconductor device factories.

On Port U15 of the VUV storage ring, a research team from the State University of New York at Stony Brook, in collaboration with the NSLS, has constructed a soft X-ray scanning microscope that is providing the first pictures of the internal structure of living cells in aqueous solutions while imparting a minimal radiation dose. Previously, electron microscopes have been employed to study cells. However, both the vacuum environment and the high radiation dose from the electrons prohibit the study of living cells, and destroy the cell's internal structure. During 1983, spatial resolutions on the 0.2 micron level have been achieved. With future improvements in resolution, and with the ability to locate the position of specific elements within a cell, this instrument may open up entirely new areas of biological research.

On a number of different UV beam lines photoemission spectroscopy has been utilized to look at electronic structures of semiconductor and metal surfaces and to study photoionization processes of gases. On Port U7, measurements on carbon films deposited on niobium before and after different annealing stages have shown a transition from an amorphous carbon layer to a graphite and, finally, a carbidic layer.

Soft X-ray excitation involving carbon 1s electrons in CO, as well as aliphatic and arimatic hydrocarbons, has been found to result in ionic fragmentation of the original molecule. The fragmentation pattern changes depending on whether the C 1s electron gets ionized or excited into a Rydberg-like orbital or into an unfilled molecular orbital.

Gas phase spectroscopy measurements on Port U11 have yielded the first photoionization excitation functions on the dimers Ar_2 and Kr_2 and the trimer Ar_3. These excitation functions display molecular Rydberg series that are closely associated with corresponding atomic Rydberg series and can be understood in a simple molecular orbital picture.

For the remainder of FY 1984 and FY 1985, significant advances are expected as the present UV beam lines continue to produce data and the EXXON beam lines on Port U1 and University of Pennsylvania/ORNL/Xerox beam lines on Port U10 begin operations. In FY 1985, initial X-ray results will be obtained from the 26 X-ray beam lines presently entering an early commissioning phase.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: A three-year, $19.7 million NSLS Phase II expansion project began in FY 1984. This project involves the development and installation of special beam lines tied to state-of-the-art undulator and wiggler insertion devices. Phase II conventional construction will expand the existing NSLS building to provide additional user laboratory and support areas and to house the entire NSLS staff in a common building.

6. For the period from the initiation of the project - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).

Answer: See attached Table.

BROOKHAVEN NATIONAL LABORATORY
NATIONAL SYNCHROTRON LIGHT SOURCE
(Dollars in Thousands)

BUDGET AUTHORITY

BUDGET PROFILE	Source of Funds	Fiscal Years 1981	1982	1983	Est. 1984	Est. 1985
OPERATIONS	Materials Sciences	$ 2,599	$ 5,098	$ 5,922	$ 7,300	$ 8,700
	Chemical Sciences	—	2,404	3,815	4,470	5,600
TOTAL OPERATIONS		$ 2,599	$ 7,502	$ 9,737	$11,770	$14,300
RESEARCH IN-HOUSE	Materials Sciences	1,390	1,738	1,946	2,305	2,426
	Chemical Sciences	1,009	1,112	1,395	1,588	1,798
	Advanced Energy Projects	136	165	104	390	90
	High Energy Physics	—	—	100	100	100
	Nuclear Physics	—	—	-	370	620
	Environmental R&D	185	273	393	443	417
OUT-OF-HOUSE	Government Agencies*	1,930	2,315	3,213	4,405	4,930
	Private Sources	1,225	1,470	1,980	3,225	3,960
TOTAL RESEARCH		$ 5,875	$ 7,073	$ 9,131	$12,826	$14,339
INVENTORIES	Materials Sciences	$ 170	$ 468	$ 250	$ 247	$ 700
CAPITAL EQUIPMENT (INCLUDES CAPITAL FOR OPERATIONS AND RESEARCH)	Materials Sciences	1,047	1,326	$ 1,296	$ 630	$ 1,035
	Chemical Sciences	288	729	899	907	623
	Advanced Energy Projects	—	—	-	160	100
	Nuclear Physics	—	—	-	400	600
	Environmental R&D	337	745	600	240	100
TOTAL CAPITAL		$ 1,672	$ 2,800	$ 2,795	$ 2,337	$ 2,458
ARAM	Materials Sciences	—	265	$ 100	$ 600	$ 1,100
GPP	High Energy Physics**	406	239	$ 611	$ 475	$ 700
IN-HOUSE ENERGY MGMT	Energy Supply R&D	—	66	$ -	$ -	$ 100
OTHER CONSTRUCTION (Phase II)	Materials Sciences	—	—	$ -	$ 2,500	$10,000

*DOE & OTHERS

NOTE: Funding levels above reflect the latest information available from the laboratory, and may very slightly from information previously provided.

7. How does the current NSLS performance compare with performance predicted prior to construction?

Answer: The UV ring began experimental operations in 1982. The VUV ring has been operated at an energy of 750 MeV, which is above the design energy of 700 MeV, with peak single-bunch currents of 400 mA, which is four times the design value. Measurements on the beam size show a horizontal emittance that is close to the design value and a vertical emittance that is within a factor of two of the design value.

The X-ray ring is in an early commissioning phase so that comparisons with design values cannot yet be made.

8. How far behind schedule is the NSLS in meeting its original performance goals?

Answer: The NSLS LINAC/Booster insertion and the UV storage ring began operations on schedule. The X-ray ring is approximately 1.5 years behind schedule.

9. What specific difficulties have been encountered in the initial operation and commissioning of the NSLS, and how are they being overcome? What are the budget implications?

Answer: Early cost-saving measures taken in the design and fabrication of the X-ray storage ring magnet supplies and diagnostic equipment resulted in inadequate performance for reliable stored beam and injection reproducibility. Improved filtering of the magnet supplies resulted in a much more stable ring and allowed higher injection currents. Additional beam position monitors have been added to the ring and additional high level software is being implemented to provide a better operator/machine interface in the measurement of closed orbits, betatron tunes, and beam currents.

10. How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?

Answer:

Outside User Research*
B/A (Thousands)

	FY 1983	FY 1984	FY 1985
Other Federal Agencies (NSF, Commerce, NIH)	1080	1168	930
Industry	3195	980	800
State Agencies	110	60	60
Total	4385	2208	1790

* DOE: FY 1983 - $922; FY 1984.- $1,090; FY 1985 - $1,240.

11. For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.

Answer:

(FTE)

FY 1981	FY 1982	FY 1983	FY 1984	FY 1985 (President's)
93	93	108	133	145

12. What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?

Answer: Full utilization of the facility would correspond to a condition where all of the UV storage ring and X-ray storage ring ports were occupied, resulting in the simultaneous operation of approximately 90 beam line (36 UV and 54 X-ray beam lines) including lines on Phase II insertion devices. The actual and estimated FY 1981 - FY 1985 utilization in operating beam lines is given below:

	FY 1982	FY 1983	FY 1984	FY 1985
UV	9	11	18	27
X-ray	0	0	18	28
TOTAL	9(10%)	11(12%)	36(40%)	55(61%)

13. **For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?**

Answer: Assuming that an average period of 40 eight hour shifts are required to start, continue and complete an experiment on a commissioned beam line, and that there are 400 shifts of operation a year on each beam line, then the estimated numbers of experiments completed at the NSLS are given below:

	FY 1983	FY 1984	FY 1985
UV:	90	110	180
X-ray	0	0	180
Total	90	110	360

14. **What is this facility's user policy?**

Answer: The NSLS is a national user facility available without charge to users. Proprietary work can be done on a full cost recovery basis, with the option for users to retain title to inventions resulting from research at the NSLS.

There are several modes of use of experimental facilities. A large number of beam lines have been designed and constructed by the 29 Participating Research Teams (PRTs). PRTs are, for the most part, user groups from outside BNL with large, long-range programs which have been approved by the NSLS Program Advisory Committee. The PRTs are given priority for up to 75% of their beam line's operational time. General users, who may have a less substantial need for the use of the facility, are scheduled for both PRT beam lines and for lines built by NSLS for the general community.

15. **For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?**

Answer: Estimates for reimbursable research are not available since arrangements are currently under negotiation with the companies involved. We roughly estimate $30,000 revenue from them in FY 1984 and $80,000 in FY 1985.

16. **What is the mechanism by which specific research proposals for experiments at the facility are considered?**

Answer: Participating Research Team proposals for instrumenting beam lines and for long-term experimental programs are submitted to the NSLS Program Advisory Committee. General users may submit proposals for single experiments or for experimental programs. General user proposals are also reviewed by the PAC.

17. How many research proposals have been submitted over the past five years, and how many of these have been approved?

Answer: There have been 35 PRT proposals over the last 5 years, 2 of which have been turned down. From June, 1983 to the present time there have been 15 general user proposals. One of these proposals has been turned down.

18. How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?

Answer: Since the beginning of UV operations in August, 1982, there have been 50 university users on the UV storage ring.

19. How many industrial researchers have utilized the facility over the past five years?

Answer: Since the beginning of UV operations in August, 1982, there have been 24 industrial researchers using the UV storage ring.

20. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer: Since the beginning of UV operations in August, 1982, there have been 7 foreign researchers using the UV storage ring.

21. How many researchers from other agencies have utilized the facility over the past five years?

Answer: There have been five researchers from other agencies since the beginning of UV operations.

22. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: A $19.7 million NSLS Phase II expansion project has been approved. This includes development and installation of special beam lines tied to state-of-the-art undulator and wiggler insertion devices. Phase II conventional construction will expand the existing NSLS building to provide additional user laboratory and support areas and to house the entire NSLS staff in a common building.

The NSLS also has given consideration to a long-range planned evolution that would include the construction and operation of a 6 GeV ring and booster synchrotron without adversely affecting the spectra of the 750 MeV or 2.5 GeV storage rings.

23. Please provide a copy of the facility's latest annual report.

Answer: A copy of the annual VUV operations report for the period September 1, 1982 - August 31, 1983 is appended.

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INFORMAL REPORT
LIMITED DISTRIBUTION

ACTIVITY REPORT ON THE NSLS VUV RING - SEPTEMBER 1, 1982 - AUGUST 31, 1983

Gwyn P. Williams

September 1983

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NATIONAL SYNCHROTRON LIGHT SOURCE
BROOKHAVEN NATIONAL LABORATORY
Associated Universities, Inc.

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I. INTRODUCTION

This report provides a summary of the first year of experimental activities on the NSLS VUV ring, that is the period September 1, 1982 to August 31, 1983. We discuss the activities of each beam line and the performance of the ring during its first operational year.

II. MACHINE OPERATION

A. History (pre September 1, 1982)

The first single turn of beam around the VUV ring was achieved on August 10, 1981. Circulating beam, r.f. capture and stacking were achieved in mid-December 1981. From December 1981 through May 1982 the ring was operated at continuously improving currents and lifetimes as the machine began to be understood and the vacuum improved. During the same period radiation surveys were made and shielding was provided where necessary to allow user access to the floor at all times, including during injection. By May, currents of around 40 m amps at 600 MeV were common, with lifetimes of 20 minutes. At that time some of the ports were opened for the first time and visible light, transmitted by windows, was viewed. In most cases the orbit and chamber alignment was such that the radiation fan was not centered on the exit port. During June and July orbit corrections were made and checked as the first beam lines were aligned (U4,U7,U9A,U9B,U14 and U15).

B. September 1, 1982 - August 31, 1983

At the start of this period beam currents of 80 mA at 600 MeV with a lifetime of 30 mins were typical. By the end of the first year we were obtaining currents of 200 mA at 750 MeV in a single bunch (300 mA maximum) with lifetimes of two hours. The source size reduced during the year from a typical vertical height (σ) of .5mm to .15mm (at 80 mA) so that we are within a factor of two of the design emittance. Thus we are now running continuously above design energy (750 MeV c.f.700 MeV) and above the design current per bunch (200 mA c.f. 111 mA) though not above the total 1 ampere design current.

There were two interruptions to operations of the machine during the year. The first, in late December 1982 was primarily for installation of additional front end components and rf antennas and involved bringing the ring up to air. The second was caused by the failure of the rf antennas. The consequences of bringing the ring up to air were fairly considerable in terms of loss of available beam time, despite the installation in Jan/Feb of the ring bakeout system. Thus, the rf cavity was separated by a pair of gate valves in March to enable it to be decoupled from the ring vacuum should future problems or improvements arise. Future plans call for the addition of water-cooled r-f antennas and a harmonic cavity to reduce bunch-bunch interactions.

C. Available Hours of Beam for Experimentation

In Tables I and II we have summarized the number of hours of beam that were available to users. We define the beam as usable if the current is greater than 10 mA and the beam was stored for more than one hour. The data from Table I are summarized in the form of a histogram in Fig. 1. Table II gives an up-to-date idea of the more recent, more reliable operation.

Several comments can be made regarding these data. During the period September 1, 1982 - May 31, 1983 the ring was running 24 hours a day so that it was necessary to have around the clock staffing on beam lines to take advantage of this beam. There were considerable waiting periods.

When the beam came on in May 1983 it was brighter (smaller source size) but there were considerable problems during May and June with orbit reproducibility. After considerable study, this problem has been almost solved, the solutions being a tune change and the inauguration of a automatic magnet hysteresis loop cycling procedure. Most (but not all) beams are now in a reproducible stable orbit. It is clearly a major advantage operationally, to be able to inject at final energy.

The last three months of the year are presented separately because they are indicative of present typical operating conditions. The machine is filled three times daily at 4:30 a.m., 8:00 a.m. and 12:00 p.m. and operation is therefore from 5:00 a.m. to about 4:00 p.m. Out of the 55 hours a week, beam is available around 47 hours or 85% of the time. Occasional extra afternoon fills explain the higher daily numbers.

III. BEAM LINE ACTIVITIES

For reference, Table III summarizes the beam lines which are planned or in operation on the VUV ring.

A. General

In September 1982 five beam lines began experimentation. By August 1983 some 12 beam lines were operating with seven more in the procurement or installation phase. These are expected to come into operation during the next year.

B. Detail of Experiments and Experimenters

In Table IV we summarize the experiments and personnel involved on a beam line by beam line basis. For each case we have listed the experiments in one column, the personnel in another. There is no cross correlation between the two columns.

IV. SUMMARY

In Figs. 1 and 2 we plot in a histogram form the beam available per week and the individual beam line histories. The growth in numbers of beamlines is evident. In Fig. 3, we show a current versus time plot for the ring taken at the very end of the period covered by this report. This is now a typical performance on a good day. For the year as a whole we had 1246 hours of available beam used by an average of 7 stations, resulting in 1090 usable shifts. Since the machine was itself in an early operational phase, the productivity per shift was not as high as it is expected to be in the future.

Commencing in the Spring of 1983 we have been requesting proposals from users and are establishing review and allocation procedures for future operation.

Table I - NSLS VUV Beam Available 9/1/82 - 8/31/83

1982							Total Monthly
September	Week	1	2	3	4		
	Beam	0	0	35	40		75
October	Week	1	2	3	4	5	
	Beam	40	40	0	0	0	80
November	Week	1	2	3	4		
	Beam	40	45	46	50		181
December	Week	1	2	3	4		
	Beam	47	46	0	0		93
1983							Total Monthly
January	Week	1	2	3	4	5	
	Beam	0	0	0	0	0	0
February	Week	1	2	3	4		
	Beam	0	0	10	18		28
March	Week	1	2	3	4		
	Beam	20	40	5	0		65
April	Week	1	2	3	4		
	Beam	0	0	0	0		0
May	Week	1	2	3	4	5	
	Beam	0	58	40	49	95	242
June	Week	1	2	3	4		
	Beam	0	55	64	50		169
July	Week	1	2	3	4		
	Beam	0	35	43	20		98
August	Week	1	2	3	4	5	
	Beam	30	44	47	45.5	48	215

NOTE: Based on U14 log book and control room records. Very approximate until June 1983. Daily records now kept.

Table II. Daily Record of Number of Hours of Beam Available in the NSLS VUV Ring During June - August 1983

	June				July				August				
Week Beginning	6	13	20	27	4	11	18	25	1	8	15	22	29
Monday	S	5.5	9	0	H	3	0	9	S	8	8.5	8.5	11
Tuesday	S	11	9	13.5	H	7	8	4	S	12.5	12	9.5	7.5
Wednesday	S	19.5	14	16	S	2.5	13	7	7	10.5	12	10	6.5
Thursday	S	12	15	9.5	S	8.5	9.5	S	12.5	5	7.5	10	11
Friday	S	7	17	10.5	S	13.5	12	S	10.5	8	7	7.5	12
Total		55	64	49.5		34.5	42.5	20	33	44	47	45.5	48

Table III. NSLS UV Beam Lines September 198

			λ(Å)	
U 1.	EXXON (Eberhardt, Hoffman, Kaldor, Kim, Stöhr, Via)	SEXAFS, ARUPS, XPS	20-2000	ERG
		INFRA-RED VIBR'TNL. SPECT.	10^4-10^6	NIM
U 2.	NSLS Diagnostics			
U 3.	LANL/SANDIA/U.CALIF/ LAWRENCE LIVERMORE (Day, Knotek, Gruner, Multhauf)	SPECTROSCOPY	12-1500	ERG
		RADIOMETRY	6-100	
U 4.	BELL LABS (Rowe, Smith, Kevan, Farrell)	A) SEXAFS/ARUPS/XPS	12-1200	PGM
		B) ARUPS	80-5000	TGM
		C) ARUPS/ABS/REFL.	400-6000	NIM
-	NSLS Free Electron Laser			
U 5.	FEL Diagnostics			
U 6.	IBM (Wilson)	LITHOGRAPHY	White	
U 7.	BNL/SUNY (Strongin, Johnson, Krummacher, Sham, Williams, Jona)	A) ARUPS/XPS/SEXAFS	15-1200	PGM
		B) GAS SOLIDS		TGM
U 8.	IBM (Himpsel, Spiller)	A) ARUPS	18-2000	TGM
		B) ARUPS	80-2500	TGM
		C) EXAFS/SEXAFS/MICR'Y.	8-100	Fresnel Zone Plate
U 9.	NSLS/BNL-CHEM. (Weston, Holroyd, Preses)	A) FLUORESCENCE LIFETIME	1050-12,000	NI
	NSLS/BNL-BIO. (Sutherland)	B) DICHROISM/FLUORESCENCE	1200-300,000	NIM
U10.	-			
U11.	NSLS/BNL-CHEM. (Grover, White)	GAS PHASE SPECTROSCOPY	300-2000	NIM
U12.	PENN/ORNL/XEROX (Plummer, Jenkins, Zehner, Salaneck)	A) ARUPS	15-1200	TGM
		B) ARUPS	80-2500	TGM
		C) INFRA-RED VIBR'TNL. SPECT.	10^4-10^6	NIM
U13.	-			
U14.	NSLS (Howells, Williams, Klaffky)	A) ARUPS/XPS/SEXAFS	15-1200	PGM
	NSLS (Hastings)	B) OPTICS R&D	8-100	DCM
U15.	NSLS/SUNY (Howells, Kirz)	TGM MONOCHROMATOR/MICROSCOPE	12-50	TGM
U16.	-			

UNASSIGNED:

TENN/NBS/ORNL (Calcott, Ederer, Arakawa)	X-RAY FLUORESCENCE	

Table IV. Personnel at NSLS VUV Ring September 1982 - August 1983 (Page 1 of 3)

Beam Line	Experiment	Personnel	Affiliation
U4	CO on Pd	M.V. Smith	Bell Labs, Murray Hill
	C core level photoemission	P.D. Johnson	Bell Labs, Murray Hill
	Sn on Ge(111)	J.E. Rowe	Bell Labs, Murray Hill
	Cu(100) surface state	S. Kevan	Bell Labs, Murray Hill
		P. Thiry	Bell Labs, Murray Hill
		P. Bennett	Bell Labs, Murray Hill
		H. Farrell	Bell Labs, Murray Hill
U5	Free Electron Laser	C. Pellegrini	NSLS/BNL
		A. Luccio	NSLS/BNL
		L. Yu	NSLS/BNL
U6	Lithography	J. Silverman	IBM, Yorktown Heights
		R. Haelbich	IBM, Yorktown Heights
		J. Warlaumont	IBM
		J. Lane	IBM
		M. Peckerar	NRL
		D. Ma	NRL
		S. Mak	NRL
U7	Photoemission, Gas phase, containing molecules	W. Eberhardt	BNL Physics
	Photoemission C	M. Strongin	BNL Physics
	Graphitic/Amorphous	D. Wesner	BNL Physics
		S. Krummacher	SUNY Stony Brook
		F. Jona	SUNY Stony Brook
		R. Carr	BNL Chem.
		T.K. Sham	BNL Chem.
		W. Eberhardt	BNL Physics
		S.L. Weng	BNL Physics
		F. Kampas	BNL, DEE
		S. Heald	BNL, DEE
		F.W. Smith	CUNY
		V. Murgai	BNL Physics
U8	Photoemission	F.J. Himpsel	IBM, Yorktown Heights
	CO or Au, Si	F.R. McFeely	IBM, Yorktown Heights
		R.A. Pollak	IBM, Yorktown Heights
		E. Spiller	IBM, Yorktown Heights
		G. Holliger	IBM, Yorktown Heights
		Y. Jugnet	IBM, Yorktown Heights
		G. Landgren	IBM, Yorktown Heights
		J. Morar	IBM, Yorktown Heights
		D. Schneisser	Fritz-Haber Inst.
		B. Reihl	IBM Zurich
		R. Parks	PINY Brooklyn
		R. Ludeke	IBM Yorktown Heights

Table IV. Personnel at NSLS VUV Ring September 1982 - August 1983 (Page 2 of 3)

Beam Line	Experiment	Personnel	Affiliation
U9A	Fluorescence Lifetimes of	J. Preses	BNL Chem.
	Hydrocarbons	R.E. Weston	BNL Chem.
	Photoconductivity in	R.A. Holroyd	BNL Chem.
	non-polar solutions	N. Zeros	BNL Chem.
	Spect. of gas phase radicals	C.R. Quick	LANL/Chem.
	Magnesium photophysics	J. Tiee	LANL/Chem.
	VUV Circ. Dichroism	J. Leventhal	U. of Missouri Phys.
	Dimethyl cadmium	C. Burkhardt	U. of Missouri Phys.
	photophysics	N. Garner	U. of Missouri Phys.
		R. Bersohni	Columbia/Chem.
		M.Q. Yang	Columbia/Chem.
		E. Premuzic	BNL/DAS
		J. Gaffney	BNL/DAS
		D. Spandau	Fla. Atl. U/Chem.
		P. Snyder	Fla. Atl. U/Chem.
U9B	VUV Circular Dichroism	J. Sutherland	BNL/Bio.
	DNA, RNA and	W. Laws	BNL/Bio.
	Virus particles	T. Coohill	W. Kentucky U.
	Photo Acoustic Spect.	C. Coray	U. of Texas, Dallas
		D. Liang	U. of Texas, Dallas
	VUVCD of Crambin	Y. Yang	U. of Texas, Dallas
	Near IR CD of photosynthesis	R. Tom	Arizona State U.
	reaction centers	D. Anjo	Arizona State U.
	Time resolved fluorescence	P. O'Hara	Arizona State U.
		P. Snyder	Fla. Atl. U.
		J. Olson	Odense U. Denmark
		T. Saarinen	Fla. Atl. U.
U11	Photoionization of O_2, rare	M. White	BNL/Chem.
	gas, free radicals (O atom),	G. Grover	BNL/Chem.
	Mixed clusters	E. Walters	U. of New Mexico
	Photoelectron spectroscopy	K. Neuman	U. of New Mexico
	Hcl + N_2O		
		B. Klemm	BNL/DAS
		F. Nesbitt	BNL/DAS
		Fernandez	U. Of New Mexico
U14	Photoemission Fe/Pd	C. Binns	U. Leicester, U.K.
		C. Norris	U. Leicester, U.K.
	Photoemission, Alloys	J. Fuggle	KFA Julich, W. Germ.
	EXAFS, spin pol. Mn.	D. Wesner	BNL/Phys.
	Ce alloys photoemission	S. Krummacher	SUNY, Stony Brook
		M. Ruckman	RPI
		E. Jensen	U. of Penn.
		B. Reihl	IBM
		R. Klaffky	NSLS
		R. Carr	BNL/Chem.
		G. Rothberg	Stevens Inst.
		K. Choudenhay	Stevens Inst.
		R. Parks	PINY, Brooklyn
		M. Denboer	PINY, Brooklyn
		G.P. Williams	BNL/NSLS
		N. Lucas	BNL/NSLS

Table IV. Personnel at NSLS VUV Ring September 1982 - August 1983 (Page 3 of 3)

Beam Line	Experiment	Personnel	Affiliation
U15	X-Ray Microscopy	J. Kirz	SUNY Stony Brook
	Lithography	H. Rarback	SUNY Stony Brook
	Diffraction	J. Kenney	SUNY Stony Brook
		D. Tierney	SUNY Stony Brook
		M. Howells	BNL/NSLS
		M. Iarocci	BNL/NSLS
		D. Sayre	IBM, Yorktown Heights
		R. Haelbich	IBM, Yorktown Heights
		R. Feder	IBM, Yorktown Heights
		B.X. Yang	SUNY, Stony Brook
		V.B. Yun	SUNY, Stony Brook

(Total of 92 people from 23 separate institutions)

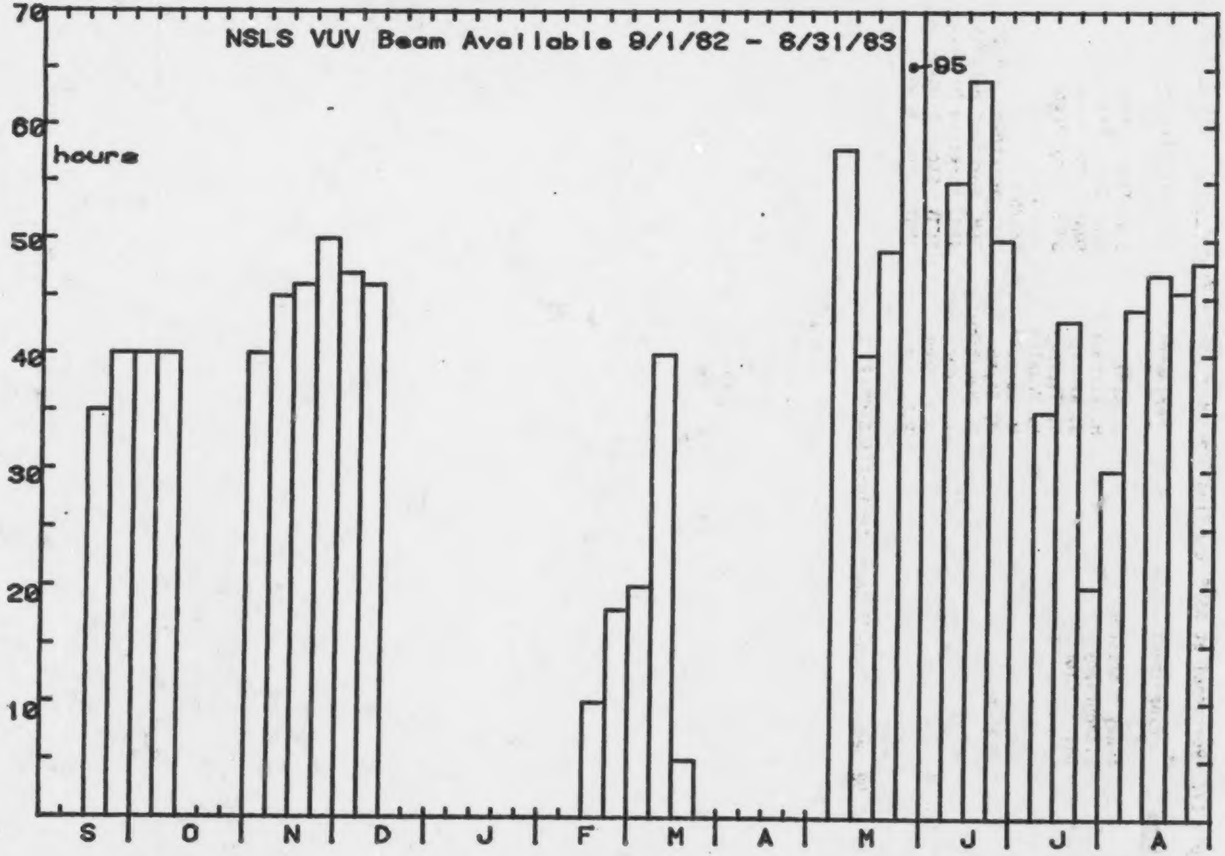
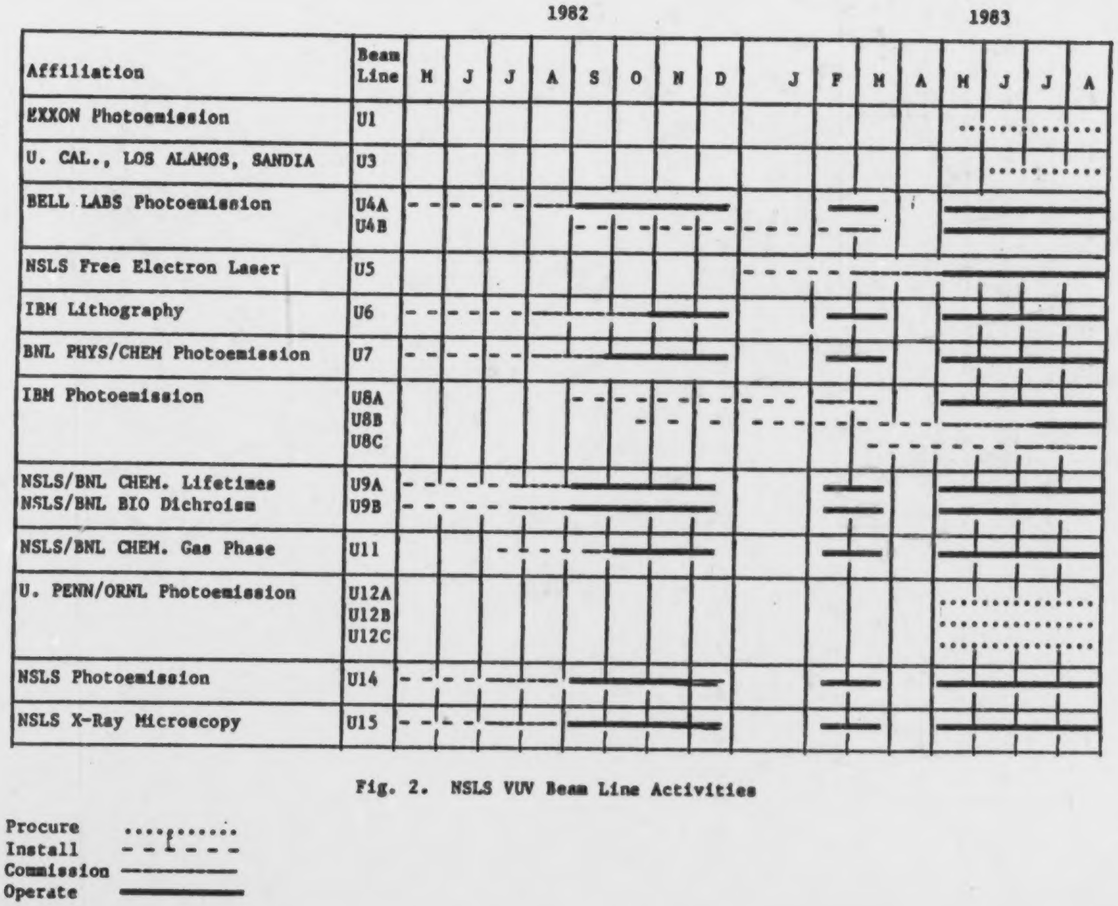


Fig. 1. Number of hours per week of usable beam at the NSLS VUV ring during the first year of operation



Affiliation	Beam Line
EXXON Photoemission	U1
U. CAL., LOS ALAMOS, SANDIA	U3
BELL LABS Photoemission	U4A U4B
NSLS Free Electron Laser	U5
IBM Lithography	U6
BNL PHYS/CHEM Photoemission	U7
IBM Photoemission	U8A U8B U8C
NSLS/BNL CHEM. Lifetimes NSLS/BNL BIO Dichroism	U9A U9B
NSLS/BNL CHEM. Gas Phase	U11
U. PENN/ORNL Photoemission	U12A U12B U12C
NSLS Photoemission	U14
NSLS X-Ray Microscopy	U15

Fig. 2. NSLS VUV Beam Line Activities

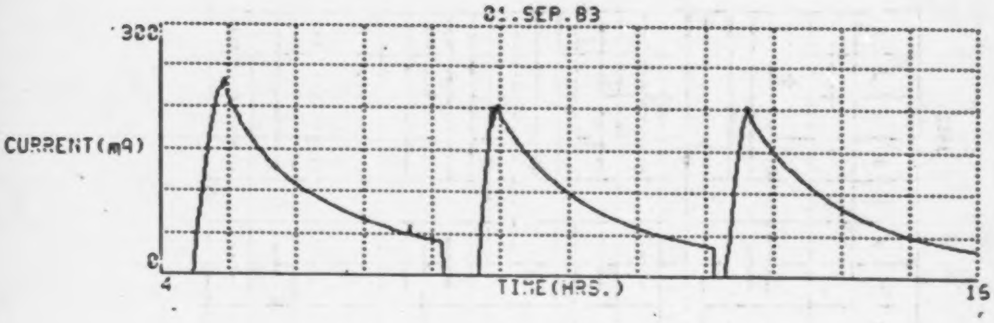


Fig. 3 - Current Versus Time Plot For NSLS VUV Ring From 04.00 Hrs. to 16.00 Hrs. on Sept. 1, 1983.

4.0 Kansas State University James R. Macdonald Laboratory

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

   Answer: The work of this laboratory is directed toward an understanding of the collision physics of highly charged ions and the intrinsic structure of such ions. In the collisions area, two velocity regimes are under study. Fast heavy ion beams moving at speeds comparable to those of the inner (K- or L-) shell target electrons are being used to investigate primary excitation, ionization and capture mechanisms. In this regime, concentration on inner shell processes for which the high charge of the nuclei dominates the motion of the electrons during the collision, makes possible the elucidation of the fundamental one electron processes responsible for the major features of the reactions and renders the corresponding theoretical descriptions tractable. Of particular interest is the continuing elucidation of mechanisms for inner-shell electron capture by fast projectiles for both symmetric and perturbative cases. In the spectroscopy area, fast heavy ions beams, collisionally stripped of all but one of their electrons, are being used to investigate quantum electrodynamic effects (Lamb Shift) in highly charged hydrogenlike systems.

   In the low velocity regime, highly charged ions with high electronic excitation levels but translation velocities much less than even outer shell electronic velocities are being generated using fast heavy-ion pumps (a technique developed at KSU and now in use in several laboratories in Europe). These slow ions are being used to investigate electron capture and capture-ionization processes at low velocity and to provide a data base for the development of theoretical descriptions of the interaction of slow highly stripped ions with simple targets such as H and He. Such processes occur in nature in the interior of fusion devices as well as in astrophysical theatres.

   Fast heavy ion beams from an accelerator are being exploited to study violent atomic processes. The use of such fast ion beams provide the only presently known way to study under controlled conditions, individual isolated collision systems involving very highly charged ions at high velocity. The slow secondary ion beams exploit the efficient transfer of electronic energy from a fast highly stripped ion to a neutral target, and have produced some of the lowest velocity data on low energy capture by multiply charged projectiles.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

   Answer: The J. R. Macdonald Laboratory is the only university-based dedicated ion-atom collisions laboratory in the country with the capability of investigating inner-shell processes which occur in violent collisions between fast heavy ions and atoms. It is the only such laboratory equipped to study ion-atom collisions involving fast heavy-ion projectiles up to about 50 MeV over most of the periodic table.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

Answer: Research Instrumentation:

- 6 MV model EN Tandem de Graaff accelerator and associated ion sources, capable of providing beams of ions ranging from H to U (not inclusive) at a maximum energy near 50 MeV; equipped with IONEX model 1610B pulsing system capable of delivering nanosecond bursts of H and heavy ions.
- 3 MV single ended Van de Graaff accelerator, capable of accelerating p and He beams.
- 150 kV accelerator capable of accelerating singly and doubly charged beams of a wide range of elements.
- PDP 11/34 data acquisition computer.
- Five electron spectrometers, three crystal x-ray detectors, 3 Si[Li] x-ray detectors, one vacuum ultraviolet spectromter; associated electronics and vacuum apparatus.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer: A sample of research highlights includes:

- The separation, via high resolution X-ray spectroscopy, of K-ionization, K-excitation and K-L capture processes and extraction of separate contributions of each to the cross section for x-ray production in collisions of 1, 2 and 3 electron projectiles with light targets. Comprehensive understanding of this process including extension to lower velocity where the interference structure becomes more marked and inclusion of double K-K transfer and will continue into 1984-85.
- The observation of interference structure in the impact parameter dependence of quasi-resonant K-K electron transfer in slow collisions of one-electron flourine with neon. Quantative theoretical understanding of these results has been achieved with atomic expansion techniques.
- The development of a secondary ion recoil source (SIRS) of very low energy highly charged ions; the first cross section measurements for electron capture below 500 eV.q.; observations of transfer ionization as an important process in low energy capture; the first measurements, via coincidence techniques of total cross sections for this process. The development of an atomic H oven for use with the SIRS source and measurements of low energy cross sections for capture from H, and H_2, by slow Ne and Ar projectiles in charge states up to + 13.
- The measurement of some of the first translational energy spectra of slow highly charged ions (up to bare nuclei of neon and fifteen times ionized argon) undergoing capture from rare gases. This work has allowed the unambiguous identification of n-values populated in such reactions. The intended continuation of this project into 1984-85 will attempt the first translational energy spectroscopy from highly charged projectiles on atomic H in our low velocity range.

- The observation of the Thomas peak in electron capture, the first direct evidence for the operation of a capture mechanism proposed in 1927 and playing an increasingly important role in capture theories developed in the 1970's; the quantitative theoretical understanding of this peak via the strong potential Born approximation without peaking approximations.

- The measurement of the 1s 1/2 Lamb Shift in hydrogenlike Cl in a fast and in a tokamak plasma.

- The identification of highly charged molecules produced in a SIRS work to identify and measure lifetimes and collisions of such molecules with simple neutral targets is expected to break new ground in low energy collisions physics and to extend into 1984-85.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: Major facility changes and additions:

- FY 1981-84, none.

- FY 1985 A proposal has been submitted to DOE and has been included in the Department's budget to upgrade the capability of the facility by:

1) adding a superconducting LINAC to the tandem, thereby roughly tripling the energy of our present beams for ions up to atomic mass of 100.

2) building a cryogenic electron beam ion source for experiments on slow, highly charged ion requiring intensities several orders of magnitude higher than provided by the SIRS.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer: Budget profiles, in units of $1,000:

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
a. Operation:	425	503	490	530	575

Total: 2523

b. In-House research: Included in the above figures. Funds are used for both operation of facility and to support in-house research.

c. Out-of-house research: Some experiments were performed at BNL, HHIRF and LBL with travel costs paid from operations funds, but were analyzed at and published from KSU.

d. Other operating expenses: None.

e. Capital equipment: No major items.

f. General plant projects: None.

g. In-House energy management: None.

h. Any other specific construction projects attributable to the facility (indicate the source of these funds.): None.

i. The source of all funds noted above is the Division of Chemical Sciences.

7. How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?

Answer: The laboratory has only received additional funding from the University.

KSU contributions to laboratory operations (in $1,000): (includes salaries and wages, plus benefits and indirect costs, and Nuclear Science Laboratory funds for periods corresponding to above contract years)

FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
156	230	194	209	226

Total: 1015

8. For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.

Answer:

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Faculty	8	8	8	8	8
Visiting Faculty & Res. Assoc.	4	4	3	2	3
Lab. Staff	3	3	3	3	3
Graduate Students	11	9	9	12	9
Total	26	24	23	25	23

9. What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?

Answer:

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Hours Beam time	2547	4764	4471	4600*	4800*
Hours down for maintenance	288	970	766	1000*	800*
Total Hrs. utilized ...	2835	5734	5237	5600	5600
"Full" Utilization**...	6000	6000	6000	6000	6000

*Based on 250 days x 24 h/day, beam on.
**Estimated

10. **For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?**

Answer: 21 experiments started, 13 experiments continued, 28 experiments completed.

11. **What is this facility's user policy?**

Answer: Users are presently invited to participate on a collaborative basis with in-house personnel. The upgraded facility will be operated on an open-to-all scientific merit basis.

12. **For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?**

Answer: None in both cases.

13. **What is the mechanism by which specific research proposals for experiments at the facility are considered?**

Answer: None exists at present since the laboratory is not a "User" facility. For the upgraded facility, a program advisory committee consisting of Kansas State and outside advisors will be set up to review experiments and allot beam time.

14. **How many research proposals have been submitted over the past five years, and how many of these have been approved?**

Answer: Does not apply.

15. **How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?**

Answer: University personnel using facility (1979-83)

Permanent faculty: 7 Visiting U. S. faculty: 5
Graduate students: 21
Undergraduate students: 27

16. **How many industrial researchers have utilized the facility over the past five years?**

Answer: 2

17. **How many researchers from foreign institutions have utilized the facility over the past five years?**

Answer: Foreign visitors using facility (1979-83): 12

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: Employees of other national laboratories or similar agencies: 3

University faculty whose major research support is from other agencies: 1

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: Included as part of the FY 1985 Appropriation is an expansion of a new booster accelerator and new low energy highly charged ion source at the laboratory. This construction, together with the existing atomic physics capability at Kansas State University, will constitute the Institute for Atomic Collision Physics. The project will involve construction and installation of (1) an advanced source of low energy highly charged ions of the CRYEBIS type and (2) a LINAC booster comprising twelve superconducting split-ring resonators. Each of these two additions will function as an adjunct to the existing tandem Van de Graaff in ways that, along with a dedicated system for high speed computation and data analysis, will have the capability to study the atomic physics of a spectrum of ions, beam time experiments, and provide a forefront environment for training young scientists and encouraging interdisciplinary cross-fertilization.

20. Please provide a copy of the facility's latest annual report.

Answer: See attached report.

A. PROGRESS REPORT

REPORTING PERIOD: 1 AUGUST 1982 THROUGH 14 SEPTEMBER 1983

Submitted to

U. S. DEPARTMENT OF ENERGY

"ATOMIC PHYSICS WITH HIGHLY CHARGED IONS"

DE-AC02-76ER02753

KANSAS STATE UNIVERSITY
DEPARTMENT OF PHYSICS
JAMES R. MACDONALD LABORATORY
MANHATTAN, KANSAS 66506

September 1983

A. PROGRESS REPORT

I. SUMMARY

This report briefly summarizes the research efforts of our group over the last year. The research group consists of nine faculty researchers, nine research associates, and thirteen graduate students. A group photograph, which appears on the next page, identifies the personnel gathered in the 72° Manhattan weather on July 14, 1983. A complete list of the laboratory personnel is given in Section II.

The laboratory had a very productive year. A total of 25 published works resulted from the research, and a total of 42 papers were presented at professional meetings and workshops. Thirteen of the oral presentations were invited talks which gives some measure of the importance accorded the Kansas State work by the scientific community. One of the Kansas State invited talks, which presented the first experimental observation of the "Thomas Peak" (Horsdal-Pedersen, Cocke and Stockli) received the hot-topic award at the ICPEAC conference in Berlin. Complete lists of the publications, abstracts and invited talks are given in Section III.

Most of the experimental work was performed with our 6 MV tandem Van de Graaff accelerator, however, many important collaborations at other laboratories have continued. Notably during the year we performed experiments at Brookhaven National Laboratory using the accel-decel tandems in order to extend the nearly symmetric F^{q+} - Ne collision studies with bare and one-electron ions to lower energies (10 MeV to 2.2 MeV). We have also performed experiments at the Oak Ridge Holifield Heavy Ion Facility to extend our study of single and double K-K transfer in nearly symmetric Cl^{q+} + Ti to energies near and above velocity match (9 MeV/amu to 15 MeV/amu). In a new effort we performed experiments at the Alcator C Tokamak at MIT to measure the $1s_{1/2}$ Lamb shift in one-electron Cl ions as produced in a plasma.

The third "Wildcorn" classic on atomic physics was held in Manhattan on October 29-30, 1982. The University of Nebraska and Kansas State University atomic physics groups met on this occasion to discuss developments in atomic physics which have occurred at the two places during the past year. New ideas often come out of this yearly event, which serves as an opportunity for our graduate students to interact with other students and faculty in an informal atmosphere. This year KSU presentations included talks by graduate students

Front Row, L to R - Dallas Kingsbury, Tom Gray, Laura Tunnell, Mike Wells, Mark Ross, Dea Richard, Shanalyn Kiger, Pat Richard, Chander Bhalla

Middle Row, L to R - Jim Legg, Basil Curnutte, S. L. Varghese, Justin Saunders, Jim McGuire, Alex Skutlartz, John Giese, C. D. Lin, Jeff Shinpaugh, Cuneyt Can

Top Row, L to R - Lew Cocke, Rudiger Brenn, Dave Hill, Bob Krause, Erik Horsdal-Pedersen, Martin Stockli, Jim Hall, Randy Dillingham, John Eck, Vince Needham

Cuneyt Can, Phil Pepmiller, and Bill Waggoner on experimental work using the KSU tandem Van de Graaff accelerator.

As discussed in our three year proposal submitted in July 1982, our research with highly charged ions has centered on several main themes. One theme is the study of one-electron processes in inelastic ion-atom scattering at "intermediate ion velocities" (ion velocities near that of the inner shell, K- or L-, electron). In these studies we have directed experiments and theory toward cases where direct and key comparisons could be made, where new processes could be investigated and where a closer look at the final state could be made to provide more information on the post-collision system. The second theme is the study of inelastic ion-atom scattering at "low velocities" using the ion-recoil method developed extensively at Kansas State. In these studies we have addressed total cross section measurements with multi-electron targets, and with one-electron targets (atomic hydrogen and alkali targets), angular distribution of projectiles following capture, and energy gain spectroscopy. The third theme is the structure of highly-ionized systems through the measurement and calculation of Auger and x-ray transition energies and transition rates.

Progress on a few selected topics is discussed below.

K-K Charge Transfer in the F-Ne System: An unexpectedly high degree of ionization of the Ne target atom was found associated with K-vacancy creating collisions, leading to He- and Li-like K Auger emitting states at certain impact parameters. To further sort this problem, the coincidence between the Ne K-Auger electrons and the recoiling Ne ions after decay were measured. For F^{q+} excitation at 0.53 MeV/u, most of the Ne ions were found left in q = 7 and 8 charge states while for F^{9+} excitation q = 8 was dominant with some q = 9 present. The corresponding Auger spectra show a dominance of hypersatellite Auger lines. This work was reported at the Berlin ICPEAC meeting this summer. The observed impact parameter dependences for single K-K transfer, which show a distinctive interference pattern at 0.23 MeV/u, were included in this report. To further investigate the transfer model, the double transfer experiment with bare ions is being run at Brookhaven National Laboratory at the lower bombarding energy using the accel-decel double tandem operation. A rich interference pattern in P(b) is anticipated for these lower energies for both single and double K-K transfer and thus allows for a more detailed test of the transient molecular orbital energies.

N-Populations in Ion-Atom Collisions: An interesting but sparcely studied quantity in ion-atom collisions is the n-distribution resulting from electron capture. We have completed a study of n-populations in F^{7+} + He and F^{7+} + Ne collisions by observing the K-Auger electron decay of the post collision F projectiles. It was found that x-ray cascading plays a big role in the observed n-distributions deduced from the K-Auger spectra. Even after correcting for cascading using a hydrogenic model it was found that at low bombarding energies (6 MeV) the n-distribution peaked at lower values than predicted by available perturbative theories. No predictions from an extended atomic basis model or molecular model are available for comparison of our experiment at present. Only the low-energy limit predicted by a classical model is available which predicts that all the capture goes to a single n-level. We hope to study this problem at lower energies in the future to see how fast the classical limit is reached in ion-atom collisions.

The $2s_{1/2} - 2p_{1/2}$ Lamb Shift: Progress has been made on the measurement of the $2s_{1/2} - 2p_{1/2}$ Lamb shift in hydrogen-like oxygen. A charge analyzing magnet has been installed on the beam line to isolate the O^{7+} beam before it enters the quenching chamber. This has reduced the background by a factor of one-third, but it has not eliminated the quench field dependence of the background. The reproducibility of the measurement has improved, partly because of the decreased background and partly because of data analysis programs which allow correction for a slight detector gain change during a measurement. The results of the first ten measurements using this scheme were reported at the DEAP meeting in May, where we also reported very preliminary results for the Lamb shift in fluorine and nitrogen. Our current results are 2212.5 ± 6.7 GHz for the Lamb shift in O^{7+} which is larger than theory but in rather close agreement with the two previous experimental determinations of this quantity.

The $1s_{1/2}$ Lamb Shift: The analysis of the $1s_{1/2}$ Lamb shift measured by x-ray spectroscopy of high velocity hydrogen-like Cl ions has progressed during the last year. The experimental result obtained from the measurement of the absolute x-ray energies gives an $S(1s) = 0.88 \pm 0.12$ eV compared to a theoretical prediction of 0.948 eV . The experimental error is still only at the 13% level, but can be improved. An improved x-ray spectrometer is presently being built for this purpose. Improved position sensitive detector systems for the x-ray spectrometer are also being investigated.

The $1s_{1/2}$ Lamb shift of Cl has also been measured by x-ray spectroscopy of the plasma from the Alcator C Tokamak at MIT. The results of these measurements yield an S(1s) = 0.85 ± 0.10 eV from the $2p_{3/2} \rightarrow 1s_{1/2}$ transition and S(1s) = 0.87 ± 0.10 eV from the $2p_{1/2} \rightarrow 1s_{1/2}$ transition. Once again, we anticipate to improve on these results in the future.

Electron Capture in Atomic Hydrogen: The electron capture by low energy highly charged neon and argon ions from molecular and atomic hydrogen has been investigated. The slow ions were produced by the recoil ion technique with energies for Ne^{q+} ($2 \leq q \leq 7$) 200-1000 eV/q and for Ar^{q+} ($2 \leq q \leq 10$) 50-3000 eV/q.

In order to study electron capture from a hydrogen atom, a thermal oven was used and measurements in an energy range 200-1250 eV/q have been completed. The results of this work will soon be submitted for publication.

Rare Gases on Li: Cross section measurements for single capture by multiply charged Ar, Ne, Kr and Xe on Li at energies between 0.1 and 1 keV per q, where q is the projectile charge state, have been completed. The cross sections are nearly independent of energy and species, depending only on q. Good agreement between the results and the absorbing sphere and classical barrier models is found. The work has just been written up for publication.

Rare Gases on He: Experimental cross section measurements for single and double electron capture and transfer ionization for Ne, Ar, Kr and Xe projectiles on He have been completed. The energy range covered was 250 to 1000 eV per q, where q is the projectile charge state. Transfer ionization is the stronger part of the double capture process, although remaining in all cases weaker than single capture. Agreement with broad-brush models for capture by highly-charged projectiles is poor. This work has been submitted for publication.

Energy-Gain Spectroscopy for Ne^{+q} on He: Translational energy spectroscopy on single capture by slow Ne^{+q} ions on He has been completed at energies of 72 to 500 eV per q and q between 3 and 10. Highly selective feeding of final states is found, with the most important selection criterion being that the appropriate crossing radius lies at a "favored" value. This value is close to the absorption radius given by the absorbing sphere model of Olson and Salop. No preferred population of a particular ℓ-value of the final electron is found beyond that accidentally occurring because of the favored crossing location. This work forms the Masters' Thesis of C. Schmeissner and is in the final stages of writing.

Capture from Li by p and He^{++}: Single capture cross sections by p and He^{++} from Li have been measured for projectile energies from 0.2 to 6 keV. These processes are of potential interest in the diagnosis of the properties of tokamak and other hot plasmas. The He^{++} cross sections seriously disagree with earlier MO calculations and some earlier experimental cross sections, but are in good agreement with recent AO calculations by Fritsch and Lin. The p cross sections are in good agreement with both old experimental data and both recent MO and AO calculations. This work is being prepared for publication.

Second Born Calculations for Electron Capture: Exact second Born calculations have been completed for electron capture. For p + He our calculations indicated that the Thomas peak should emerge at energies above several MeV/amu. This was confirmed by an experiment done at Kansas State, where the Thomas peak was observed for the first time, giving a structure in qualitative, but not quantitative agreement with theory, including the recent and powerful strong potential Born theory. In collaboration with Professor N. C. Sil, visiting from Calcutta, India, a technique was developed to evaluate terms in the SPB theory to an accuracy consistent with the SPB approximation itself. Thus, peaking approximations previously used to evaluate the SPB amplitudes were avoided. The resulting cross sections are in quantitative agreement with the shape of the observed Thomas peak. Furthermore, with this new technique, it is now possible to calculate cross sections for capture to and from excited states in the SPB approximation.

Work has also been completed showing how the Thomas peak emerges for electron capture in systems of various charges in exact second Born calculations, using computing facilities at the Hahn-Meitner Institute in Berlin. Also, it has been shown that Wick's theorem is satisfied in the SPB approximation with full peaking, lending additional support to the credibility of this approximation.

Work has also been done investigating two electron transitions (the simplest of multi-electron transitions) in atomic collisions. In particular an explanation has been given for a factor of two difference in the double ionization of helium by electrons and protons at quite high projectile velocity. This difference has been attributed to an interference between two competing (a first and a second Born) mechanisms for double excitation and ionization. Suggestions for further experimental investigations have been presented.

While the Glauber approximation has been quite successful in reproducing experimental results for atomic collision cross sections (e.g., direct Coulomb ionization of H by heavy ions), the theory contains an apparent inconsistency for inelastic scattering, raising a question about the integrity of the Glauber approximation. For inelastic scattering by heavy projectiles this apparent inconsistency has been resolved lending credence to Glauber calculations for ion-atom collisions.

II. JAMES R. MACDONALD LABORATORY PERSONNEL

Faculty

Chander P. Bhalla, Professor

C. Lewis Cocke, Professor

Basil Curnutte,[1] Professor

John S. Eck, Professor

Tom J. Gray, Professor

Siegbert Hagmann, Assistant Professor

James C. Legg, Professor

James H. McGuire, Professor

Patrick Richard, Professor; Principal Investigator

Visiting Faculty and Research Associates

Rüdiger Brenn, Visiting Professor, Albert-Ludwigs-Universität, Freiburg, W. Germany

James Hall, Research Associate

Erik Horsdal-Pedersen, Visiting Scientist, University of Aarhus, Aarhus, Denmark

Stefan Kelbch, Research Assistant, University of Frankfurt, Frankfurt, W. Germany

Horst Schmidt-Böcking, Visiting Professor, University of Frankfurt, Frankfurt, W. Germany

N. C. Sil, Visiting Professor, Indian Association for the Cultivation of Science, Calcutta, India

Martin Stockli, Research Associate

Thomas W. Tunnell, Visiting Scientist, N.O.R.D.A., NSTL Station, Mississippi

S. L. Varghese, Visiting Professor, University of South Alabama, Mobile, Alabama

Research Collaborators for Experiments Performed at Other Laboratories

B. Johnson, K. Jones, and M. Meron, Brookhaven National Laboratory, N. Y.

P. Cowan, R. Deslattes, and R. LaVilla, National Bureau of Standards, Washington, D. C.

G. Alton, D. Gregory, C. Jones, P. Miller, C. Moak, and P. Pepmiller, Oak Ridge National Laboratory, Oak Ridge, Tennessee

L. Bridwell, Murray State University, Kentucky

C. Sofield, Harwell, England

E. Källne and J. Källne, Smithsonian Astrophysical Observatory and Alcator C Tokamak Laboratory, Massachusetts

Research Collaborators Cont'd

R. Mann, G.S.I., Darmstadt, W. Germany

E. Justiniano and R. Schuch, Universität Heidelberg, Heidelberg, W. Germany

Laboratory Staff

Ron Gifford, Technician Assistant

Walter Heimbach, Draftsman

Dave Hill,[1] Machine Shop Foreman

Robert Krause, Accelerator Engineer

Dea Richard, Secretary

Mark Ross,[1] Electronics Engineer

Mike Wells, Accelerator Technician

Graduate Research Assistants

Cuneyt Can

Randy Dillingham, Ph.D. granted in 1983, presently Research Scientist at Kansas State University

John Giese

Vince Needham

Joal Newcomb, Ph.D. granted in 1983, present address: NORDA, NSTL Station, Mississippi 39529

A. Rahman Omar

Philip Pepmiller, Ph.D. granted in 1983, present address: Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830

Justin Saunders

Chris Schmeissner

Jeff Shinpaugh

Alexander Skutlartz

Laura Tunnell

William Waggoner

Undergraduate Research Assistants

Jeff Dauber

Neufito Luis Fernandes

Shanalyn Kiger

Mike King

David Kingsbury

Robbin Kletke

Jeff Krause

Alan Lankford

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[1] Supported by Kansas State University

III. PUBLICATIONS

Journal Publications for period 1 August 1982 - 14 September 1983

Exact Second Born Electron Capture for p + He
P. R. Simony, J. H. McGuire and J. Eichler
Phys. Rev. A 26, 1337 (1982)

Measurement of the Lamb-Shift in Hydrogen-like Oxygen
Basil Curnutte, C. Lewis Cocke, and R. D. DuBois
Nucl. Instr. & Methods 202, 119 (1982)

A Study of Transfer Excitation in F^{8+} + He, Ne and Ar Collisions
Philip L. Pepmiller, Patrick Richard, J. Newcomb, R. Dillingham, J. M. Hall, Tom J. Gray, and M. Stockli
IEEE Vol. NS-30, 1002 (1983)

X-Ray Satellite Lines from Doubly Excited States of Heavy Ions with Few Electrons Produced in Ion-Atom Collisions
H. Tawara and Patrick Richard
Nucl. Instr. & Methods 205, 597 (1983)

Satellite Structure in the 2pσ Molecular Orbital Transitions in Slow Heavy Ion Collisions
Martin P. Stockli
IEEE, Vol. NS-30, 916 (1983)

Fusion Cross Sections for ^{9}Be + ^{40}Ca
J. S. Eck, A. R. Omar, J. R. Leigh and T. R. Ophel
Phys. Rev. A 27, 1807 (1983)

Systematics of Single and Double K-Shell-Vacancy Production in Titanium Bombarded by Heavy Ions
James Hall, Patrick Richard, Tom J. Gray, J. Newcomb, P. Pepmiller, C. D. Lin, K. Jones, B. Johnson and D. Gregory
Phys. Rev. A 28, 99 (1983)

Electron Capture Collisions Involving Low-Energy Highly-Stripped Projectiles
C. L. Cocke, T. J. Gray, E. Justiniano, C. Can, B. Waggoner, S. L. Varghese, and R. Mann
Physica Scripta T3, 75 (1983)

Charge Asymmetry Dependence of X-Ray Transitions into the 2pσ Quasi-molecular Orbital Emitted in Slow Heavy Ion Collisions
Martin P. Stockli
Spectral Line Shapes, Vol. 2, 1033 (1983)

K-Shell Auger Rates for Multiply-Ionized Atoms II. Fluorine
C. Can, T. W. Tunnell and C. P. Bhalla
J. Electron Spec. and Related Phenomena 27, 75 (1982)

Experimental Observation of the Thomas Peak in High-Velocity Electron Capture by Protons from He
E. Horsdal-Pedersen, C. L. Cocke, and M. Stockli
Phys. Rev. Letters 50, 1910 (1983)

Lifetimes and Fluorescence Yields of States Produced in Heavy Ion-Atom Collisions
C. P. Bhalla
IEEE Vol. NS-30, 1093 (1983)

Theoretical Lifetimes, X-Ray Transition Energies and Fluorescence Yields for Double K-Vacancy Configurations of Multiply-Ionized Fluorine
C. Can and C. P. Bhalla
IEEE Vol. NS-30, 1090 (1983)

Theoretical X-Ray Transition Energies and Fluorescence Yields for Multiply-Ionized Oxygen
C. P. Bhalla
IEEE Vol. NS-30, 1097 (1983)

A Review of Recoil Ion Physics
Tom J. Gray and C. L. Cocke
IEEE Vol. NS-30, 937 (1983)

Electron Capture Cross Sections for Low Velocity Ne^{q+}($q = 2-6$) Incident Upon Atomic Hydrogen
Tom J. Gray, C. Can, J. M. Hall, L. Tunnell, and S. L. Varghese
IEEE Vol. NS-30, 895 (1983)

An Experiment Apparatus for Low Energy High Charge State Heavy Ions to Study Collisions on Atomic Hydrogen
C. Can, Tom J. Gray, J. M. Hall, L. N. Tunnell and S. L. Varghese
IEEE Vol. NS-30, 943 (1983)

Surface Spectroscopy Using High Energy Heavy Ions
B. L. Doyle, P. S. Peercy, Tom J. Gray, C. L. Cocke and E. Justiniano
IEEE Vol. NS-30, 1252 (1983)

Capture of Ar K-Shell Electrons by Protons
E. Horsdal-Pedersen, C. L. Cocke, J. L. Rasmussen, S. L. Varghese, and W. Waggoner
J. Phys. B 16, 1799 (1983)

The Strong Potential Approximation with Non-Orthogonality Terms
J. H. McGuire
IEEE NS-30, 1100 (1983)

Quasi-Resonant K-K Charge Exchange in F-Ne Collisions
S. Hagmann
IEEE NS-30, 928 (1983)

Double Ionization of Helium by Protons and Electrons at High Velocities
J. H. McGuire
Phys. Rev. Letters 49, 1153 (1982)

Charge-State Dependence of Fluorine K X Rays in F-Ne Collisions
Philip L. Pepmiller and Patrick Richard
Phys. Rev. A 26, 786 (1982)

Interpretation of Second Born Amplitudes in Electron Capture
J. H. McGuire, P. R. Simony and O. L. Weaver
Phys. Rev. A 26, 1109 (1982)

Electron Capture by and Electron Excitation of Two-Electron Fluorine Ions Incident on Helium
M. Terasawa, Tom J. Gray, S. Hagmann, J. Hall, J. Newcomb, P. Pepmiller, and Patrick Richard
Phys. Rev. A 27, 2868 (1983)

Papers Accepted for Publication

Proper Derivation of the Glauber Approximation for Inelastic Scattering by Heavy Particles
J. H. McGuire
J. Phys. B

Electron Capture by Metastable Projectiles on He and Ne
J. Newcomb, T. R. Dillingham, J. Hall, S. L. Varghese, P. L. Pepmiller, and P. Richard
Phys. Rev. A

Application of Wick's Theorem in the Strong Potential Approximation
J. H. McGuire
Phys. Rev. A

Exact Second Born Calculations for Electron Capture for Systems with Various Projectile and Target Charges
J. H. McGuire, P. R. Simony and J. Eichler
Phys. Rev. A

Strong Potential Born Calculations for Electron Capture
J. H. McGuire and N. C. Sil
Phys. Rev. A

Abstracts

Electron Capture Cross Sections for Low Velocity Ne^{q+} (q = 2,3,4,5 & 6) Incident Upon Atomic Hydrogen
Tom J. Gray, C. Can. J. M. Hall, L. N. Tunnell, and S. L. Varghese
BAPS 27, 800 (1982)

An Experimental Apparatus for Low Energy High Charge Heavy Ions to Study Collisions on Atomic Hydrogen
C. Can, Tom J. Gray, J. M. Hall, L. Tunnell and S. L. Varghese
BAPS 27, 800 (1982)

Charge Transfer in Ne^{8+}-Ne Collisions Between 1 and 100 eV Impact Energy
S. Hagmann, C. L. Cocke, P. Richard, A. Skutlartz, H. Schmidt-Böcking and R. Schuch
Thirty-Fifth Gaseous Electronics Conference
Dallas, Texas (October 1982)

Theoretical X-Ray Transition Energies and Fluorescence Yields for Multiply-Ionized Oxygen
C. P. Bhalla
BAPS 27, 803 (1982)

Quasi-Resonant K-K Charge Exchange in F-Ne Collisions
S. Hagmann
BAPS 27, 758 (1982)

Satellite Structure in the 2pσ Molecular Orbital Transitions in Slow Heavy Ion Collisions
Martin Stockli
Post-deadline abstract - Denton meeting

Theory of Electron Capture at High Velocity
J. H. McGuire
DOE Contractors' Meeting, ORNL, April 1983

Delta Electron Emission in 10 MeV F^{q+} + Ne
A. Skutlartz and S. Hagmann
Kansas Academy of Sciences (1983)

Electron Capture Cross Sections for Low Velocity Highly Charged Ions (LEHQ) on Atomic and Molecular Hydrogen
T. J. Gray, C. Can, L. Tunnell, J. M. Hall, and S. L. Varghese
BAPS 28, 940 (1983)

The ^{40}Ca(^{7}Li,^{6}Li)^{41}Ca Reaction at E(^{7}Li) = 45 MeV
John S. Eck, K. W. Kemper, and T. R. Ophel
BAPS 28, 717 (1983)

The ^{9}Be + ^{9}Be Nuclear Interaction: Elastic, Inelastic, and Reaction Cross Sections at E(^{9}Be) = 35,40,45,50 and 55 MeV
A. R. Omar, John S. Eck, T. R. Ophel and J. R. Leigh
BAPS 28, 715 (1983)

Measurement of the $1s_{1/2}$ Lamb Shift in Hydrogen-Like Chlorine
M. P. Stockli, Patrick Richard, R. Mann, R. D. Deslattes, P. Cowan, R. E. LaVilla, B. Johnson, K. Jones, M. Meron, and K. Schartner
BAPS 28, 781 (1983)

Formation of Doubly Excited Two Electron Ions During F^{8+} + He, Ne or Ar Collisions
Philip L. Pepmiller, Patrick Richard, J. Newcomb, J. M. Hall, T. R. Dillingham, and M. Stockli
BAPS 28, 777 (1983)

An Anisotropy Measurement of the Lamb-Shift in Hydrogen-like Oxygen
Basil Curnutte and C. Lewis Cocke
BAPS 28, 789 (1983)

Systematics of Projectile K-Auger Electron Production by Bare, One, and Two Electron Ions
T. R. Dillingham, J. Newcomb, J. Hall, P. Pepmiller, and Patrick Richard
BAPS 28, 777 (1983)

Double Ionization of Helium by p^+ and e^- at High Velocities
J. H. McGuire
BAPS 28, 815 (1983)

K-Auger Hypersatellite and Satellite Spectra for He-, Li- and Be-like Ne after 0.53 MeV/u F^{9+} Impact Excitation
S. Hagmann, C. L. Cocke, P. Richard, A. Skutlartz, H. Schmidt-Böcking, and R. Schuch
BAPS 28, 816 (1983)

Measurements of Single Electron Capture Cross Sections in Collisions Between Low Energy Highly Charged Rare Gas Projectiles and Neutral Li Atoms
W. T. Waggoner, C. L. Cocke, M. Stockli and S. L. Varghese
BAPS 28, 778 (1983)

Measurement of n-Populations for Electron Capture by F^{7+} Projectiles
J. Newcomb, Patrick Richard, T. R. Dillingham, J. M. Hall, Philip L. Pepmiller and S. L. Varghese
BAPS 28, 777 (1983)

Triple Difference Probabilities for Delta-Electron Emission in 10 MeV F^{9+} + Ne
A. Skutlartz and S. Hagmann
BAPS 28, 816 (1983)

Observation of the "Thomas" Peak in Electron Capture from He by Fast Protons
C. L. Cocke, E. Horsdal-Pedersen and M. Stockli
BAPS 28, 778 (1983)

Detailed Test of Optical Potentials for the Transfer Reactions $^{40}Ca(^{7}Li, ^{6}Li, ^{6}He)$
C. P. Sanderson, K. W. Kemper, and J. S. Eck
Notre Dame Nuclear Meeting

Electron Capture Cross Sections for Low Velocity Ne^{q+} and Ar^{q+} Ions on Atomic and Molecular Hydrogen (50 eV/q to 3000 eV/q)
Tom J. Gray, C. Can, L. Tunnell, J. M. Hall and S. L. Varghese
ICPEAC XIII (1983)

Charge Asymmetry Dependence of X-Ray Transitions into the 2pσ Quasi-Molecular Orbital Emitted in Slow Heavy Ion Collisions
Martin P. Stockli
6th Int'l Conf. on Spectral Line Shapes, Boulder, Colorado (July 1982) p. 88

Collision Broadening of the 2pσ Molecular Orbital Transitions in Cu-X-Collisions
Martin P. Stockli
Int'l Conf. on X-Ray and Atomic Inner-Shell Physics
Book of Abstracts, p. 205 (1982)

Interferences Due to Competing Mechanisms for Double Excitation and Ionization of Atoms at High Velocities
J. H. McGuire
Volume of Contributed Papers, XIII ICAP (Berlin, 1983) p. 166

Exact Second Born Calculations for Electron Capture
J. H. McGuire, J. Eichler and P. R. Simony
Volume of Contributed Papers, XIII ICAP (Berlin, 1983) p. 499

Resolution of the Glauber Inconsistency for Inelastic Collisions by Heavy Particles
J. H. McGuire
Abstracts of papers of the XIII ICPEAC Meeting (Berlin, 1983) p. 362.

A Weighted Curve Fitting Program for the HP 67/97 Calculator
Martin P. Stockli
BAPS 28, 787 (1983)

Invited Talks

Lifetimes and Fluorescence Yields of States Produced in Heavy Ion-Atom Collisions
C. P. Bhalla
BAPS 27, 806 (1982)

A Review of Recoil Ion Physics
Tom J. Gray
BAPS 27, 789 (1982)

Transfer Excitation Studied by High Resolution Spectroscopy: F^{8+} + He, Ne and Ar Leading to Doubly-Excited Satellite X-Ray Transitions
P. Richard
U. S./Japanese Cooperative Science Seminar, Book of Abstracts,
p. 49 (1983) Honolulu, Hawaii

High and Low Velocity Electron Capture
C. L. Cocke
U. S./Japanese Cooperative Science Seminar, Book of Abstracts,
p. 25 (1983) Honolulu, Hawaii

Some Possibilities and Limitations of a SIRS Source for Investigating Low-Energy Capture Reactions
C. L. Cocke
DOE Atomic Physics Program Contractors' Workshop, Oak Ridge National
Laboratory, April 1983, Program and Abstracts p. 47.

A Study of the $1s_{1/2}$ Lamb Shift in Hydrogen-like Chlorine
Patrick Richard
DOE Atomic Physics Program Contractors' Workshop, Oak Ridge National
Laboratory, April 1983, Program and Abstracts p. 63.

K Auger Spectroscopy in K-K Charge Transfer
Siegbert Hagmann
DOE Atomic Physics Program Contractors' Workshop, Oak Ridge National
Laboratory, April 1983, Program and Abstracts p. 80.

Recoil Ions - Production and Uses
C. L. Cocke
Argonne National Laboratory Workshop on "Atomic Physics with Fast Heavy-Ion Beams," January 1983, p. 161

X-Ray Spectroscopy with Fast Heavy-Ion Beams
Patrick Richard
Argonne National Laboratory Workshop on "Atomic Physics with Fast Heavy-Ion Beams," January 1983, p. 33.

Energy Gain Spectroscopy and e-Capture Cross Sections for Low Energy Highly Charged Ions on He and H_2
Tom J. Gray
ISIAC VIII, Castle Nijenrode, Breukelen, The Netherlands (1983)

The Production and Use of LEHQ Recoil Ions in Atomic Physics Investigations
Tom J. Gray
International Workshop on Cross Sections for Fusion and Other Applications, College Station, Texas (1982)

Thoughts on the Future of K to K Charge Transfer
Siegbert Hagmann
International Workshop on Cross Sections for Fusion and Other Applications, College Station, Texas (1982)

Experimental Observation of the Thomas Peak in Electron Capture
E. Horsdal-Pedersen, C. L. Cocke and Martin Stockli
XIII ICPEAC, Berlin (1983)

IV. LABORATORY OPERATIONS

Tandem Van de Graaff Accelerator

During the reporting period August 1, 1982 through September 14, 1983, the tandem Van de Graaff accelerator at Kansas State University was operated 4471 hours. The two inclined field tubes which were installed in January 1982 in the low energy end of the accelerator have accumulated 7274 hours of operation and the two inclined field tubes installed in December 1974 in the high energy end of the accelerator have accumulated 26,249 hours of operation.

Down time for this reporting period totaled 766 hours of which 288 hours were used for the replacement of the charging belt and 120 hours were used for diagnostics on our low energy incline field tubes. The remaining 358 hours were used for periodic maintenance.

On-Line Computer

During the last year of operation, a number of minor problems occurred with our PDP 11/34A computer.

- It was discovered that six of the original disk packs had become physically warped and were intermittently rubbing the head. These disk packs were discarded.
- Intermittent computer crashes, which we believe are associated with a microprocessor in the operator's console have occurred. This problem has not yet been identified.
- Three stepping motors in our line printer burned out, with associated damage in the circuitry providing a holding current to the motor. This holding current has been dropped to a safer value.
- We have experienced intermittently an obscure problem in which a low-priority program making many computations errs when run with a higher-priority data-taking program. The definite source of these errors has not been established, though the executive program is suspected.

The Apple microcomputer terminal mentioned in the last progress report is being used to make graphs and simple fits to data; and a program has been written which lets the Apple monitor the accelerator beam current and dial a user's telephone when the beam current falls below a preset level for a preset interval.

Data-taking using CAMAC electronics continues to expand and further expansions of CAMAC capabilities are planned.

B. SCOPE OF WORK

There are no significant changes to the current scope of work or methods of accomplishment. Therefore, the scope of work remains the same as given in the original three-year proposal.

C. FINANCIAL REPORT

The proposed funding levels requested in this IFR are the same as originally anticipated for FY84. This IFR is therefore for $530,000 for work from February 15, 1984 through February 14, 1985.

There will be no unexpended funds for the current funding period.

5.0 Lawrence Berkeley Laboratory National Center for Electron Microscopy

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

Answer: Microstructural characterization of materials at, or close to, the atomic level is being carried out on both the Atomic Resolution Microscope (ARM) and the 1.5 MeV High Voltage Electron Microscope (HVEM). The complementary capabilities of the microscopes are furthermore exploited in many studies. At 1.5 MeV, relatively thick specimens are transparent to electrons thus allowing bulk structural changes to be followed in-situ during heating, cooling or straining treatments, either in high vacuum or in controlled gaseous environments. Applications of this type include studies of basic phase transformation mechanisms, solar cell degradation, catalyst particles, nuclear waste storage materials and semiconductor devices. The same specimens may be imaged at the atomic level in the ARM prior to, and following, such treatments to deduce the atomic structural rearrangements which have occurred. Such studies provide an understanding of the relation between structure, segregation to and electronic properties of, dislocations in semiconductors, catalyst and solar cell performance, and the factors governing the microstructural stability of many other metallic, ceramic, magnetic and semiconductor alloys.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

Answer: The National Center for Electron Microscopy is unique because of the assortment of instruments and expertise which it provides in one centralized location, fully dedicated to the microstructural and microchemical characterization of materials. It is the only facility in the world to offer an Atomic Resolution Microscope which has better than 1.8 Å point-to-point resolution over a 400 kV to 1000 kV voltage range and a ± 40° biaxial goniometer stage.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

Answer:

Date	Instruments	Key Features	Characterization
1982	KRATOS 1.5MeV Electron Microscope	Resolution 3 Å (pt-pt) environmental cell; hot, cold stages	50-80 hrs/week 150-1500 kV range in 100 kV steps and continuously variable. Max beam current 70 amp/cm^2. 3mm diameter specimens
1984	JEOL 1 MeV Atomic Resolution Microscope (ARM)	Resolution 1.7 Å (pt-pt) over full voltage range. Ultra-high resolution goniometer stage, ± 40° biaxial tilt with height control	50-80 hrs/week 400 kV 1 MeV LaB$_6$ filament 3 mm diameter specimens

Date	Instruments	Key Features	Characterization
1970	Hitachi 650 kV Electron Microscope	General purpose resolution 20 Å environmental cell straining stage	Installed in 1969. Max. voltage 650 kV conventional HVE
1981	JEOL 200CX Electron Microscope	Dedicated high-resolution 2.4 Å (pt-pt) U.H. resolution goniometer stage only	200 kV only LaB_6 2.3 mm diameter specimens
1984	200 kV dedicated Analytical Electron Microscope	X-ray and energy-loss spectrometers microdiffraction (CEB)	100 kV-200 kV state of-the-art resolution
1984	400 kV Analytical Electron Microscope (requested)	Above capabilities over extended voltage range and foil thickness	

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer:

1981: The facility was still under construction.

1982: The HVEM became operational mid-way through 1982. During its first 6 months of use its major research applications were; studies which showed certain Ni-Ti alloys were rendered amorphous under electron irradiation; an investigation of cross-sectioned semiconductor devices that pin-pointed the defects responsible for premature failure; and direct observation of the reduction process in nickel oxide crystals. Also, high resolution images of a grain boundary in molybdenum provided the first direct experimental support for the "O"-lattice model.

1983: An in-situ oxidation study of stainless steel demonstrated varying rates of attack in the grain boundary regions and matrix which was related to alloy composition variations. The mechanism of crystallization of amorphous films of ion-implanted gallium-arsenide was studied in-situ. Relative stabilities of metastable carbide phases in platinum-carbon alloys were obtained from hot stage experiments. Atomic resolution images of precipitates in a molybdenum-hafnium-nitrogen alloy directly verified a new model for precipitate growth by a vacancy mechanism.

1984: The mechanism of degradation of the Cu_2S/CdS solar cell was identified by high resolution electron microscopy to be loss of Cu by propagation of a 1/4[010] stacking disorder. Poor cell performance was also associated with the formation of a 50 Å thick transition phase between the p-type absorber and n-type collector layers. Continuing in-situ studies of the development precipitate morphologies in iron-base alloys have provided further support for a new crystallographic theory of precipitation. Atomic resolution images which discriminate atomic sites and types have been obtained from barium titanate crystals. The defects that arise in response to stress concentrations in semiconductor device structures are being characterized using the HVEM. The microstructures of whiskers of silicon carbide and silicon nitride in the as-grown condition are being characterized in the HVEM.

Atomic resolution images of the core structures of undissociated and decorated dislocations in silicon and GaAs are anticipated. Initial results on the direct imaging of atomic positions in zeolites are also expected.

1985: In-situ studies of the controlled oxidation of Al alloys, annealing of deformed Si and GaAs and precipitation in iron-base alloys are expected to be completed. Atomic resolution microscopy of intercalated compounds, doped GaAs, zeolites, and ceramic powder-processed materials and grain boundaries in face-centered cubic metals is also planned.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer:

1982: Installation of the 1.5 MeV HVEM microscope and the JEM 200CX high resolution feeder microscope were carried out. Construction of the ARM silo was also completed during this year.

1983: Both the 1 MeV ARM and the JEM 200CX analytical electron microscope were acquired and the installation of specimen preparation equipment (ion beam thinner) and image analysis computer terminals was completed.

1984: The ARM Support Laboratory (ASL) has been completed this year and image analysis hardware is to be installed. All relocation of equipment (darkrooms, evaporators, ultrasonic specimen cutters, diamond saw, feeder microscope) should be completed by year's end.

1985: The microscopes in NCEM will be modified for on-line image simulation and analysis, and a new medium-voltage (~400kV) analytical electron microscope should be added during this year. Spectrometer development for the high voltage microscopes will also be carried out.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer:

B/A (dollars in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Facility Operation	505	767	880	1090	1400
[1]In-House Research*	0	30	114	130	260
[1]Out-of-House Research+	0	40	80	170	340
Other Operating Expenses	0	0	0	0	0
Capital Equipment	238	80	115	140	279
General Plant	0	0	0	0	0
In-House Energy Management	0	0	0	0	0
Construction	3152	1955	463	270	100

All funds are Materials Sciences in origin except where noted.

* In-house research is supported through the Materials and Molecular Research Division.

+ Out-of-house research is funded from a wide variety of agencies including DOE, NSF, NIH, DOD, and Industry.

1 These figures were estimated on the basis of salary plus overhead per shift worked multiplied by a factor of three for specimen preparation and interpretation of results. A factor of four was used for outside researchers to take account of travel expenses.

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer: No money was provided for the facilities or operations by other agencies.

8. **For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.**

Answer:

FTE	FY 1983	FY 1984	FY 1985
Principal Investigator(s)*	3	3	3
Postdoctoral(s)	0	1	3
Other Scientists	2	3	4
GSRAs (Graduate Students)	1	3	3
Support Staff	5	6	8

* Varying percentages of time.

9. **What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?**

Answer:	1981	1982	1983	1984	1985
HVEM*	N.A.	N.A.	80	75	75
ARM**	N.A	N.A	N.A.	30	80

Figures for Percent Utilization.

* High Voltage Electron Microscope
** Atomic Resolution Microscope

"Full" utilization of any single microscope occurs at an 80% figure, based upon the fact that one day per week is needed for routine service and maintenance. Through FY 1984, the standard working shift has been 10 hours per day, resulting in 40 hours per week for a "full" utilization condition.

During 1985 the microscopes will run 16 hours per day, in either one or two shifts, resulting in a "full" utilization condition of 64 hours per week.

10. **For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?**

Answer:

HVEM Since 1983 there have been, and will continue to be, a total of approximately 30 experiments per year on a continued basis. New experiments will be added as older ones are finished.

ARM Starting in 1984 there will be a total of approximately 20 experiments per year. New experiments will be added as older ones are finished.

11. **What is this facility's user policy?**

Answer: Any qualified electron microscopist who proves scientific validity of his experiment as well as the need for the unique instrumentation provided here may use the facility.

12. **For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?**

Answer: Users are not charged for the use of the NCEM facility unless experiments involve proprietary data requiring confidentiality. The only reimbursable research during this period was done by Mobil Oil Company, 10 hours in January 1984 reimbursing the facility in the amount of $2,310. We do not foresee any further reimbursable research in the near future.

13. **What is the mechanism by which specific research proposals for experiments at the facility are considered?**

Answer: Proposals are submitted in which a brief description of the research is provided. These are screened and judged by a Steering Committee composed of eleven members, eight of whom are not members of the Facility. They are from industry and other academic institutions.

14. **How many research proposals have been submitted over the past five years, and how many of these have been approved?**

Answer:	HVEM:	70 submitted: 67 approved, 3 rejected
	ARM:	20 submitted: 19 approved, 1 rejected

15. **How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?**

Answer: Approximately 44 university personnel (i.e. faculty and students) have utilized the facility over the past five years.

16. **How many industrial researchers have utilized the facility over the past five years?**

Answer: Over the past five years approximately 8 industrial researchers have utilized the facility.

17. **How many researchers from foreign institutions have utilized the facility over the past five years?**

Answer: Over the past five years, 3 researchers from foreign institutions have utilized the facility.

18. **How many researchers from other agencies have utilized the facility over the past five years?**

Answer: Four principal investigators have been funded by other agencies.

19. **What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?**

Answer: There are many potential future development possibilities for the existing National Center for Electron Microscopy, but there are currently no specific plans to undertake any of them beyond the construction activities identified in the FY 1985 budget request.

20. **Please provide a copy of the facility's latest annual report.**

Answer: At the present time NCEM is part of the Materials and Molecular Research Division and does not issue separate reports. The section of the MMRD annual report which describes NCEM activities is attached together with the Users' Guide which is updated periodically.

MMRD Annual Report 1983

Account: 4062
Contact Person: U. Dahmen, ext. 5516

National Center for Electron Microscopy

Gareth Thomas, Ronald Gronsky and Kenneth H. Westmacott, Investigators

Introduction. The National Center for Electron Microscopy (NCEM) aims to provide state-of-the-art facilities for electron-optical characterization of materials and to develop techniques of imaging, interpretation, and microanalysis.

The very high cost of modern instruments dictates time-sharing centers where facilities, support, and staff are all available. The center, available to all qualified researchers, is built around two new microscopes, each housed in its own three-story silo. Installed in 1982, the High Voltage Electron Microscope (HVEM), accelerating electrons to energies of 1.5 million electron volts (MeV), is the most powerful microscope of its kind in the U.S. The Atomic Resolution Microscope (ARM), installed in 1983, operates in the 0.4 to 1.0 MeV range. It offers the highest resolution in the world, with 1.6Å already proved.

The two microscopes will enable materials scientists and biologists to study samples under the most realistic conditions possible and to distinguish individual atoms even in closely packed metallic and ceramic structures.

Support facilities at the center include 100- and 200 keV transmission electron microscopes, microanalytical instruments, equipment for preparing specimens, image analysis devices, and computer simulation hardware and software.

The facility will be fully operational in 1984. The Seventh International Conference on High Voltage Electron Microscopy was held at Berkeley on August 16-19, 1983, with approximately 100 participants (see LBL Rept. No. 16031).

The Center is guided by a Steering Committee whose present non-LBL members are: Drs. J. Hren (U. of Florida), Chairman, W. L. Bell (General Electric Company), M. Gibson (Bell Labs.), D. Howitt (U.C. Davis), M. Simnad (AMES, La Jolla), J. C. H. Spence (Arizona State University) and A. Taylor (Argonne National Laboratory).

1. 1.5MeV High Voltage Electron Microscope

K. H. Westmacott

Since the modifications to the accelerator tube bleeder resistor chain were completed, the microscope has been performing extremely well. The high voltage instability problem is completely resolved and full working day operation at 1500kV is now routine.

Of the 67 research proposals received to date, about one-half are currently active. Research on the instrument runs the gamut from phase transformation studies in metals, ceramics and minerals, to semiconductor devices and amorphous metal investigations to biological and medical science applications.

Usage statistics for 1983 show an average weekly utilization of greater than 80% (excluding the three weeks down time for the modifications). The ratio of materials science to biological science use is now about 6:1.

A listing of the new proposals approved during 1983 is given in Table I.

Table. I. HVEM Research Proposals

Principal Investigator	Affiliation	Title
A. Evans (Crumley)	UCB, Mat. Sci. and Min. Engrg.	Thin-foil studies of ceramics
R. Ayer	Exxon	Electron microscopic analysis of formation of surface oxide films during high temperature oxidation
T. Cass	Hewlett Packard	Defect structures in semiconductor devices
G. Brooks	UCB, Physical Education Dept.	Adaptations in skeletal muscle mitochondrial morphology with endurance exercise
C. E. Warble	CSIRO, Australia	Pd/MgO Reaction Study
R. Gronsky (T. Sands)	LBL, MMRD	In-situ study of the degradation of $Cu_{2-x}S/CdS$
R. Stoller	UCSB, Chem. and Nucl. Engrg.	Influence of a preinjected helium on void swelling in a model austenitic alloy
E. Dratz	UCSC, Nat. Sci.	High voltage TEM studies of ocular melanin in the retinal pigment epithelium
E. Dratz	UCSC, Nat. Sci.	Energy dispersive spectroscopy of inclusion bodies in the thin sections of retinal pigment epithelial cells
R. Spohr	GSI Darmstadt	HVEM studies of latent nuclear tracks
G. Reid	Hewlett Packard	HVEM studies of stress-induced defect generation in CMOS-VLSI devices
J. Dash	Portland State Univ., Physics	Electrodeposition of chromium and copper in magnetic fields
J. Dash	Portland State Univ., Physics	Phase transformations induced by high pressures and temperatures in a ballistic compressor

J. Clarke (Pelz)	UCB, Physics	Investigation of 1/f noise in metal films due to defects
J. W. Morris, Jr. (Katagiri)	UCB, Mat. Sci. and Min. Engrg.	Fatigue crack propagation mechanisms of structural alloys at cryogenic temperatures
G. Thomas (Kwok)	UCB, Mat. Sci. and Min. Engrg.	Micromechanisms of wear
M. A. Meyers	New Mexico Inst. Mining and Tech.	A metallurgical study of dynamic fracture in metals
A. Evans (Inoue)	UCB, Mat. Sci. and Min. Engrg.	Phase transformation toughening in 3.2%MgO-ZrO_2
H. J. Ralston, III	UCSF	Three-dimensional structure of thalamic neurons
A. K. Mukherjee	UCD, Mech. Engrg.	In-situ HVEM studies on cavitation 7475 aluminum alloys
G. Thomas (Wasynczuk)	UCB, Mat. Sci. and Min. Engrg.	Characterization of precipitates within cementite
A. Searcy (Kim)	LBL, MMRD	In-situ study of thermal decomposition of $Mg(OH)_2$
G. Thomas (Krishnan)	UCB, Mat. Sci. and Min. Engrg.	Atom location by channelling inversion voltage phenomena
R. Wenk (McTigue)	UCB, Geology	Dislocation properties of silicate garnets

1.1 HVEM Facility Improvements

Several improvements in the capabilities for in-situ studies are in progress. At present hot stage work in the environmental cell is severely limited by the inability to attain high temperatures in the flowing gas due to heat dissipation problems. Furnace-type hot stages reach only ~800°C while platinum strip heaters are notoriously unreliable. An improved direct heating grid design is being constructed to overcome some of these deficiencies. A second problem, that of heating of the environmental cell apertures by heat conduction through the gas is being reduced by a modification that directly cools the cell walls.

In response to a developing demand, an order for a Birmingham-type* ambient temperature-double tilting-straining stage has been placed. This is a well tested design that uses a piezoelectric device, or optional manual drive, for imparting stress to the specimen. A further advantage is the minimal specimen movement ensured by driving both jaws of the straining stage. When this stage is on line, attempts will be made to add a heating capability to extend its utility to a wider variety of materials studied.

The present video system has allowed considerable experience to be gained and the factors limiting the quality of video reproduction has been assessed. A new sophisticated system is now planned which will be integrated into the entire Center computer network.

A modification to the camera vacuum system is also in progress which will allow a significant reduction in the time to resume operation following a change of cassettes. When this improvement is implemented, two-shift operation of the HVEM will commence.

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*Birmingham University, U. K.

1.2 Typical Examples of HVEM Work in Progress (These examples are from work in progress from UCB-LBL investigators. Abstracts of all research are approved by the Steering Committee and copies are on file.)

1.2.1. The Transformation Aragonite —> Calcite and Calcite —> Lime Observed In-Situ by HVEM, H. R. Wenk* and J. W. McTigue, Jr.* The transformation between calcite and the related phases aragonite and lime is of interest to the geologist as well as the ceramist. Aragonite is the high temperature form of $CaCO_3$ while calcite is its stable low temperature form. It is known that the two crystal structures are derivatives of the fcc and hcp structure, respectively and that the transition involves a 10% change in volume. However, the mechanism of transformation is unknown. This applies equally to the decomposition of calcite to lime. The loss of CO_2 in this reaction ($CaCO_3 \rightarrow CaO + CO_2$) causes a very large volume change resulting in a highly porous reaction product.

Because of the sensitivity to radiation damage by 100keV electrons, HVEM is necessary to study the details of the transformation mechanisms. At the same time the available heating stages provide high stability and good control in the temperature range of the transformations (400-500°C). The aragonite to calcite transition was found to occur very rapidly with a boundary sweeping across the foil erasing twins and dislocation substructures in aragonite, a feature typical of massive transformations in metal alloys. Videotape recordings will allow a closer examination of this rapid transformation.

The transformation of calcite to lime proceeds more slowly maintaining a topotaxial relationship of parallel close packed planes in the two lattices. This suggests a gradual loss of CO_2 from the Ca^{++} framework. The developing porosity begins as thin platelets with a tendency to align parallel to (0001) calcite.

*Geology Department, UC Berkeley.

1.2.2. HVEM In-Situ Study of Precipitate Dissolution in a Pt-C Alloy, D. Ackland, U. Dahmen and K. H. Westmacott. Two metastable precipitates, α and α' are known to form in rapidly quenched and aged dilute platinum-carbon alloys. Both are thin plates on {001} planes and microdiffraction has revealed that the structure of α is a precursor to the body-centered tetragonal α' carbide. The kinetics of plate shrinkage were measured from sequences of micrographs recorded during in-situ isothermal annealing, as shown in Fig. 1.1. Both types of precipitate were found to exhibit linear dissolution kinetics, but in distinctly different temperature regimes. The α plates shrank at an average rate of $0.02 nms^{-1}$ at 450°C while the measured rate for α' was $0.005 nms^{-1}$ at 515°C, indicating a much greater stability of α'. These results are in good agreement with ex-situ and bulk coarsening data which suggest the reaction is controlled by vacancy diffusion. Further measurements combined with careful calibration of the microscope hot stage promise to yield results which may be used quantitatively to determine activation energies.

1.2.3. Structure of Electrodeposited Chromium, R. M. Fisher† and K. H. Westmacott. Chromium coatings, 5-100 μm in thickness are widely used to improve corrosion and wear resistance. Their brightness, hardness and tendency to crack depend on plating conditions. The effect of plating conditions on the columnar grain structure of electrodeposited chromium, the nature of the residual stresses, and the distribution of entrapped plating solution (H_2CrO_4) have been studied using high voltage and scanning electron microscopy and electron and ion beam microanalytical techniques. Electrodeposited chromium is characterized by (1) the occurrence of large tensile stresses in the exposed surface side that often result in extensive cracking and peeling from the substrate and (2) a substantial amount of entrapped plating solution.

†Assoc D... Industry Participation

~~†Industry Participation Officer, CAM, LBL~~

High voltage electron microscopy has revealed that the microstructure consists of highly-elongated columnar grains. A representative 1000kV transmission electron micrograph of a stripped and ion-thinned sample of hard, bright chromium plating is shown in Figure 1.2. The 0.1μm diameter grains (in cross section) exhibit a strong <111> fiber texture along their columnar axis and contain a dislocation density of about $2 \times 10^{11}/cm^2$. Heating electrodeposited chromium at 800 to 900°C results in recrystallization, 1 to 2% shrinkage of the film, the relief of tensile stresses through the formation of numerous cracks, the evolution of hydrogen and the formation of Cr_2O_3 particles. It appears that the void space in the unequilibrated intercolumnar grain boundaries contains oxygen and hydrogen (possibly as adsorbed H_2O), resulting in a tendency for the film to shrink as the hydrogen is absorbed by the highly dislocated metal lattice.

This study has provided the first direct information about the exceptionally high stresses in electro-plated chromium.

1.2.4. In-Situ Epitaxial Regrowth of Ion-Implanted GaAs, T. Sands, D. K. Sadana[†], J. Washburn and R. Gronsky. Gallium arsenide is becoming an increasingly attractive semiconducting material for electron and opto-electronic device applications. However, the science of GaAs processing lags far behind the science (and art) of silicon device processing. In particular, doping by ion implantation is a much more complex process for GaAs than for Si. In this study, high voltage (HVEM) and high resolution (HREM) electron microscopy are applied to the study of the annealing behavior of GaAs layers that have been amorphized by the implantation process. HREM images of cross-section specimens show that the as-implanted amorphous-crystalline transition region is finite in width and consists of small pockets of crystalline material in an amorphous matrix (Fig. 1.3). Furnace annealing at 400°C results in epitaxial regrowth of this transition region. However, once the interface becomes simply-connected, stacking fault bundles are nucleated. Fig. 1.4 shows the effect of in-situ annealing (20 min., 400°C) in the HVEM on the sample imaged in Fig. 1.3. Note that the epitaxial regrowth has terminated at the end of the transition region. Further in situ HVEM work will be directed toward determining the kinetics of this epitaxial-regrowth process.

[†] Microelectronics Center of North Carolina, Research Triangle Park, NC 27709

1.2.5 A Generalization of Atom Location by Channelling Enhanced Microanalysis. K. M. Krishnan and G. Thomas. The technique of atom location by channelling enhanced microanalysis (ALCHEMI) has limitations in practical application. A generalization of this technique, with the underlying idea that additional relationships can be generated by performing these experiments at an appropriate number of orientations depending upon the stoichiometry of the original compound has been developed. The precise number of orientations required to solve the distributions in a whole class of related compounds is expressed in terms of the stoichiometry of the original compound along with the alloying additions.

Fig. 1.1 Sequences of micrographs showing precipitate shrinkage at linear rate during in-situ isothermal annealing in the HVEM. (a) field of α precipitates shrinking at $0.02nms^{-1}$ at 725K; (b) field of α' precipitates shrinking at $0.005nms^{-1}$ at 788K. (XBB 830-11124)

Fig. 1.2 Dark field TEM (1000kV) showing cross-section of columnar grids in hard, bright electrodeposited chromium. (XBB 830-11123)

Fig. 1.3 Cross-sectional HREM image (<110> orientation) of amorphous-crystalline transition region in as-implanted GaAs (450keV Se^+ into (100) GaAs, dose $1 \times 10^{14}/cm^2$, room temperature) (XBB 830-9399)

Fig. 1.4 Sample of Fig. 1.3 before and after in situ annealing in HVEM (20 min., 400°C). Buried amorphous layer in as-implanted material is 190nm wide. (XBB 830-11122)

2. Atomic Resolution Microscope

R, Gronsky

Installation of the Atomic Resolution Microscope (Fig. 2.1) was completed and the instrument formally accepted on July 25, 1983. Nearly all performance specifications were exceeded by the ARM at its LBL site; most notably its imaging resolution was demonstrated to be 0.16 nm at 1 MeV accelerating potential (Fig. 2.2). This result clearly establishes the unique capabilities of this instrument for resolving individual atoms in densely-packed engineering materials.

Careful attention has since been given to calibration of the microscope and the establishment of routine user operating conditions. Among these activities has been the simplification of astigmatism correction, enhancement of brightness, determination of proper alignment procedures and identification of lens settings for convergent beam electron diffraction (Fig. 2.3).

The ARM will be open to the user community during January of 1984, and occupation of the new support laboratory will follow shortly. This addition to Building 72 will house three support microscopes, specimen preparation equipment and image analysis hardware.

2.1. High Resolution Study of Plate Precipitates in a Mo-Hf-N Alloy, R. Gronsky, K. H. Westmacott and U. Dahmen.

Mo-Hf-N is a mixed substitutional/interstitial alloy forming plate-shaped precipitates of HfN on {001} planes of the Mo matrix. HfN has the NaCl crystal structure and is related to the bcc Mo matrix by the Bain correspondence which for this particular combination of lattice parameters describes an invariant plane strain, a simple extension normal to the precipitate habit plane. Like other precipitates formed by an invariant plane strain transformation, HfN has been reported to grow by a ledge mechanism. The large volume change of about 40% that accompanies the transformation must be accommodated by lattice vacancies. If stacking violations of {001} planes are to be avoided, vacancies must condense in double layers. This will place discrete limits on the optimal precipitate thicknesses and ledge heights. To test the model, high resolution structure images of the HfN plates were obtained on the ARM operated at 1MeV. An example of an image in the symmetrical $<100>_{Mo}$ orientation is shown in Fig. 2.4. The thick plate of fcc HfN is viewed precisely edge-on and is readily distinguished from the Mo matrix. Two features are clearly evident: (1) the precipitate-matrix interface is atomically smooth and (2) the precipitate contains no faults in the stacking sequence. This evidence supports the proposed model and the resulting plate is predicted to have an 8% interstitial strain field.

2.2. High Resolution Microscopy Investigation of the ZrO_2-ZrN System, G. van Tendeloo* and G. Thomas.

The ZrO_2-ZrN system has been investigated using different electron microscopy techniques. In the range between 2.5 mol.% and 75 mol% ZrN, an incommensurate modulated structure is formed having a rhombohedral $R\bar{3}$ symmetry based upon the $Zr_7O_{11}N_2$ structure which is isostructural to $Zr_5Sc_2O_{13}$. The modulation is most probably due to pseudoperiodic composition fluctuations of nitrogen with respect to oxygen. The final structure can be described as a completely coherent mixture of pure Zr_7O_{14} layers alternating with $Zr_7O_{11}N_2$ layers perpendicular to the rhombohedral threefold axis. The incommensurability arises from local deviations in spacing and/or orientation of these layers. Monoclinic precipitates imbedded in this rhombohedral matrix are characterized with the help of high resolution electron microscopy combined with optical microdiffraction. Configurations which minimize the strain energy are common (Fig. 2.5).

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Fig. 2.1. Console level view of the ARM. Large ion pump mount is visible on the upper left of the column; diagonal tube attached to left of specimen chamber is mass spectrometer head. Specimen exchange rod is attached horizontally to the right, and the manual controls for the goniometer descend the front of the column. The terminal at the lower right addresses all memory locations, digital console display and text field on micrograph negatives. Console controls are efficiently interfaced to the CPU, which reduces their total number. (CBB 839-8469)

Fig. 2.2. Optical diffractograms from high resolution image~~s~~ of ~~(a) gold particles showing discrete 0.23, 0.20 and 0.14nm reflections (left) and (b)~~ amorphous Si ~~(right)~~ at Scherzer defocus, 1000kV. The diffractogram halo ~~in (b)~~ is continuous out to a resolution limit of 0.16nm.

~~((a) XBB 836-5045~~ ~~(b)~~ XBB 836-5044)

Fig. 2.3. Convergent beam electron diffraction pattern from a Si specimen in [011] orientation showing higher order Laue zone lines within the central disc. (XBB 836-5048).

Fig. 2.4. High resolution image of HfN precipitate plate in a molybdenum matrix. The precipitate is seen to be three unit cells thick (see outlines), free of stacking faults, and bounded by an atomically smooth interface. (XBB 839-7867).

Fig. 2.5. High resolution observation of heavily twinned monoclinic ZrO_2. All variants have a common c-axis parallel to the electron beam. The orientation of the axes as determined from HREM and optical diffraction is indicated. (XBB 838-7156).

1983 Publications and Reports

Refereed Journals

1. R. G. Regnier, N. Q. Lam and K. H. Westmacott, "Microstructural Transitions in Pt-C Alloys during High-Voltage Electron Microscope Irradiation", J. Nucl. Mat. 115, 286 (1983).
2. R. Kilaas and R. Gronsky, "Real Space Image Simulation in High Resolution Electron Microscopy", Ultramicroscopy 11, 289 (1983).
3. G. van Tendeloo, K. T. Faber and G. Thomas, "Characterization of AlN Ceramics Containing Long Period Polytypes", J. Mat. Sci. 18, 525 (1983).
4. M. Sarikaya, J. W. Steeds and G. Thomas, "Lattice Parameter Measurements in Retained Austenite by CBED", Proc. EMSA, 1983, p. 206 G. W. Bailey (ed.), San Francisco Press, Inc.
5. G. van Tendeloo and G. Thomas, "Electron Microscopy Investigations of the ZrO_2-ZrN System. I. Formation of an Incommensurate Superstructure Zr-O-N", Acta Met. 31, 1611 (1983).
6. G. van Tendeloo, L. Anders and G. Thomas, "Electron Microscopy Investigation of the ZrO_2-ZrN System. II. Tetragonal and Monoclinic ZrO_2 Precipitation", Acta Met. 31, 1619 (1983).
7. R. Gronsky and G. Thomas, "Instrumentation at the NCEM: The Atomic Resolution Microscope", Proc. EMSA, 1983, p. 310, G. W. Bailey (ed.), San Francisco Press, Inc.

LBL Reports

8. K. Krishnan, P. Rez, R. K. Mishra and G. Thomas, "Determination of the Specific Site Occupation of Rare Earth Additions in $Y_{1.7}Sm_{0.6}Lu_{0.7}Fe_5O_{12}$ Thin Films by the Orientation Dependence of Characteristic X-ray Emissions", Materials Research Society Meeting, Boston, MA, November 13-17, 1983, LBL-16884.

9. K. Krishnan, L. Rabenberg, R. K. Mishra and G. Thomas, "Site Occupation of Ternary Elements in $Sm_2(CoTM)_{17}$ Compounds", J. Appl. Phys. in press, LBL-16874.

10. G. van Tendeloo and G. Thomas, "High Resolution Microscopy Investigation of the ZrO_2-ZrN System", J. Amer. Cer. Soc., in press (Proc. Int. Conf. ZrO_2--1983: Stuttgart), LBL-16240

11. K. Krishnan, P. Rez and G. Thomas, "Effect of Voltage on the Orientation Dependence of Electron Induced Characteristic X-ray Emissions", Proc. 7th HVEM Conf., Berkeley, CA, 1983, p. 365, LBL-16144.

Other Publications

12. Proceedings of the 7th International Conference on HVEM, Berkeley, August 16-19, 1983, R. M. Fisher, R. Gronsky and K. H. Westmacott (eds.), LBL-16031.

13. U. Dahmen, P. Ferguson and K. H. Westmacott, "HVEM Studies of Precipitate Morphology Symmetries", Proc. 7th International Conference on HVEM, Berkeley, CA, R. M. Fisher, R. Gronsky and K. H. Westmacott (eds.), p. 315 (1983).

14. D. Ackland, U. Dahmen and K. H. Westmacott, "HVEM In-Situ Studies of Precipitate Coarsening and Dissolution in a Pt-C Alloy", Proc. 7th International Conference on HVEM, Berkeley, CA, R. M. Fisher, R. Gronsky and K. H. Westmacott (eds.), p. 319 (1983).

15. R. M. Fisher and K. H. Westmacott, "Structure of Electrodeposited Chromium", Proc. 7th International Conference on HVEM, Berkeley, CA, R. M. Fisher, R. Gronsky and K. H. Westmacott (eds.), p. 323 (1983).

16. P. Ferguson, U. Dahmen and K. H. Westmacott, "In-Situ Study of γ' Precipitation in Fe-N", Proc. 7th International Conference on HVEM, Berkeley, CA, R. M. Fisher, R. Gronsky and K. H. Westmacott (eds.), p. 227 (1983).

17. R. Gronsky, "Electron Microscopy at Atomic Resolution", Proc. of Materials Research Society Symposium on Electron Microscopy of Materials, W. Krakow (ed.), North Holland (in press), LBL-16937.

18. R. Gronsky, "High-Resolution Transmission Electron Microscopy", Treatise on Materials Science and Technology, Vol. 19, Part B, H. Herman (ed.), Academic Press, 1983. LBL 11243

19. U. Dahmen and K. H. Westmacott, "A TEM Analysis of Repeated Precipitation on Climbing Dislocations in Al-4Cu", 11th Western Regional Meeting of Electron Microscopists, Pacific Grove, CA 1983, LBL-16382.

20. P. Ferguson, U. Dahmen and K. H. Westmacott, "Morphological Aspects of α''-$Fe_{16}N_2$ Precipitation in α-Iron", 11th Western Regional Meeting of Electron Microscopists, Pacific Grove, CA, 1983. LBL 16661.

Invited Talks:

21. K. H. Westmacott and R. Gronsky, "National Center for Electron Microscopy", TMS/AIME Meeting, St. Louis, MO, October 1982.

22. R. Gronsky, "Developments in Electron Microscopy", Forum of the Solid State Sciences Committee, National Academy of Sciences, Washington, D. C. February 8-9, 1983.

23. K. H. Westmacott, "Applications of HVEM in the Study of Precipitation Reactions", AIME Meeting, Atlanta, February 1983.

24. R. Gronsky and G. Thomas, "Atomic Resolution Microscopy of Materials", TMS/AIME and ASM/MSD Joint Symposium on Metals Research at User-Oriented National Facilities, TMS/AIME Meeting, Atlanta, Georgia, March 6-10, 1983.

25. R. Gronsky, "Electron Microscopy: the State of the Art", Industrial Liaison Program, Fifth Annual Conference, U. C. Berkeley, March 9-10, 1983.

26. R. Gronsky, "National Center for Electron Microscopy", Invited Poster Session on National Facilities of Importance to Condensed Matter Physics, American Physical Society Annual Meeting, Los Angeles, CA, March 22, 1983.

27. G. Thomas, "The National Center for Electron Microscopy, Berkeley", Special Meeting of the Indian Institute of Science and Technology, Delhi, India, April 25, 1983.

28. G. Thomas, HVEM and its Applications in Materials Science", Bombay Atomic Energy Research Center, Bombay, India, April 27, 1983.

29. R. Gronsky, "Imaging Atomic Structure in the TEM", Department of Chemical and Nuclear Engineering Special Symposium, U. C. Santa Barbara, Santa Barbara, CA, May 2, 1983.

30. G. Thomas, "The NCEM Berkeley--Fulfillment of a Nine-Year Project", Keynote Speaker, Biannual Conf. Northern and Southern California E.M. Societies, Asilomar, May 11, 1983.

31. G. Thomas, "Characterization of Ceramics", J.S.P.S. Subcommittee, Tokyo, Japan, May 19, 1983.

32. U. Dahmen, "Applications of HV and HR Electron Microscopy", Metals and Welding Conference, San Francisco, CA, May 1983.

33. R. Gronsky, "Instrumentation and Interpretation in Atomic Resolution Microscopy", EUCHEM Conference on High Resolution Electron Microscopy in Solid State Chemistry, Royal Swedish Academy of Sciences, Stockholm, Sweden, June 12-16, 1983.

34. G. Thomas, "National Center for Electron Microscopy", Electron Microscopy of Ceramics, Toulouse, France, July 1983.

35. G. Thomas, "Instrumentation at the NCEM; ARM", EMSA Conf., Phoenix, Arizona, August 6-12, 1983.

36. R. Gronsky , "Atomic Resolution Microscopy", Materials Science Seminar, Department of Materials Science and Mineral Engineering, U. C. Berkeley, November 1, 1983.

37. G. Thomas, "The NCEM and the Approach to Atomic Resolution of Solids", Diamond Jubilee Celebrations, Varanasi, India, Plenary Lecture, November 1983.

38. G. Thomas, "The National Center for Electron Microscopy--Development of Materials Research", Plenary Lecture, New England Society for Electron Microscopy, December 7, 1983.

Fig. 1.1

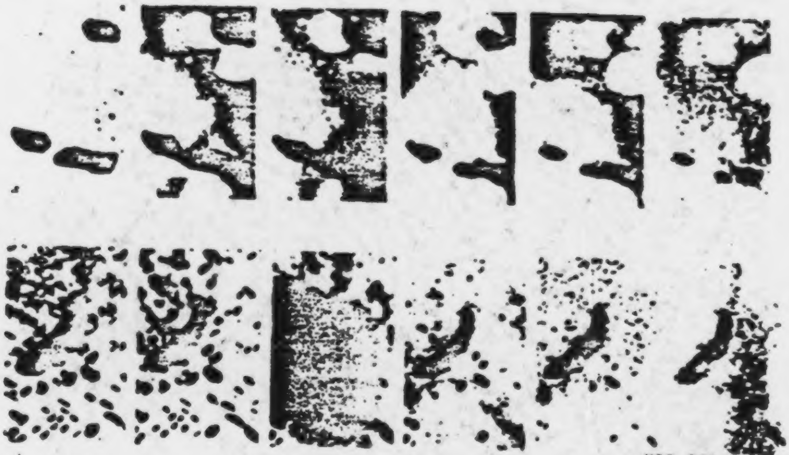
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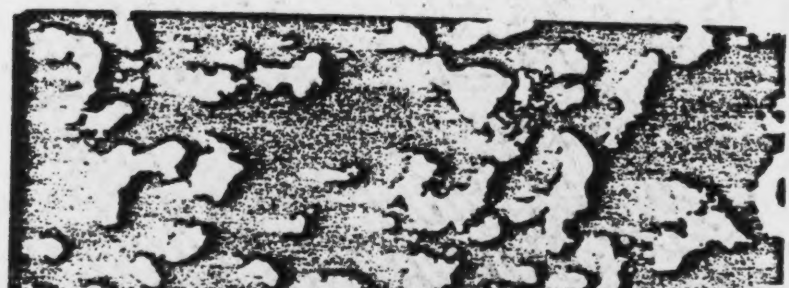
Fig. 1.2



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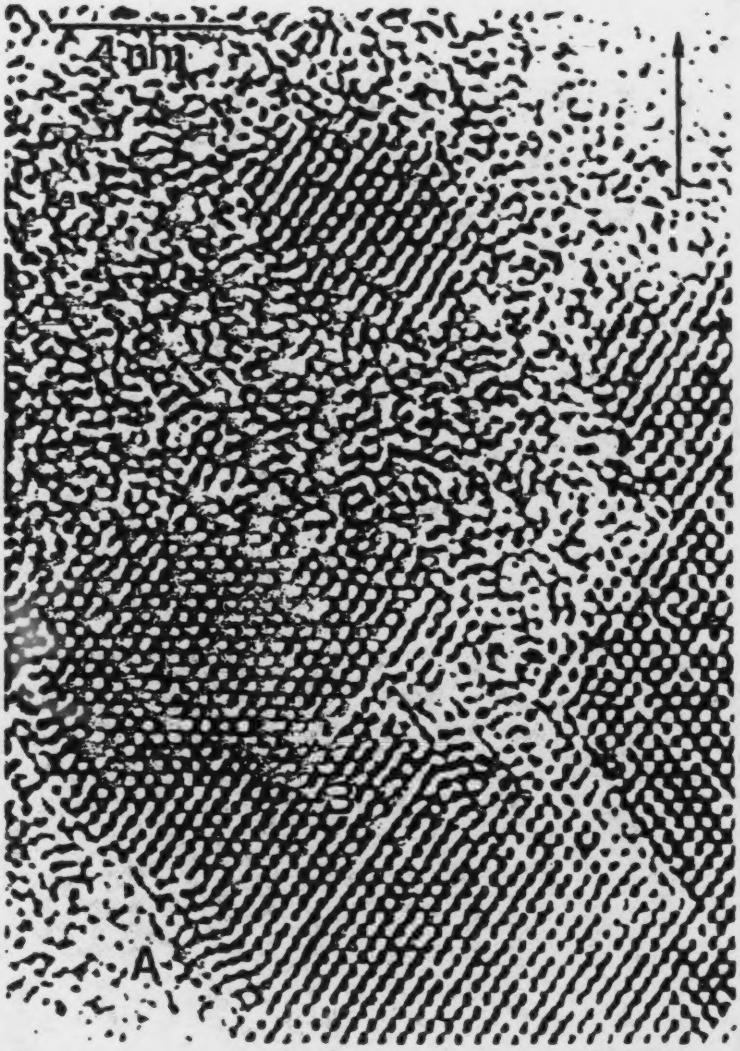
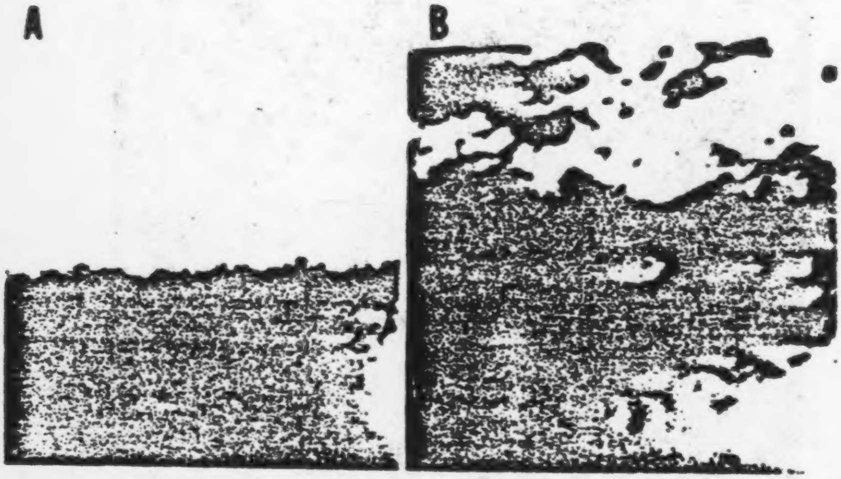


XBB 830-9399

Fig. 1.3

Fig. 1.4



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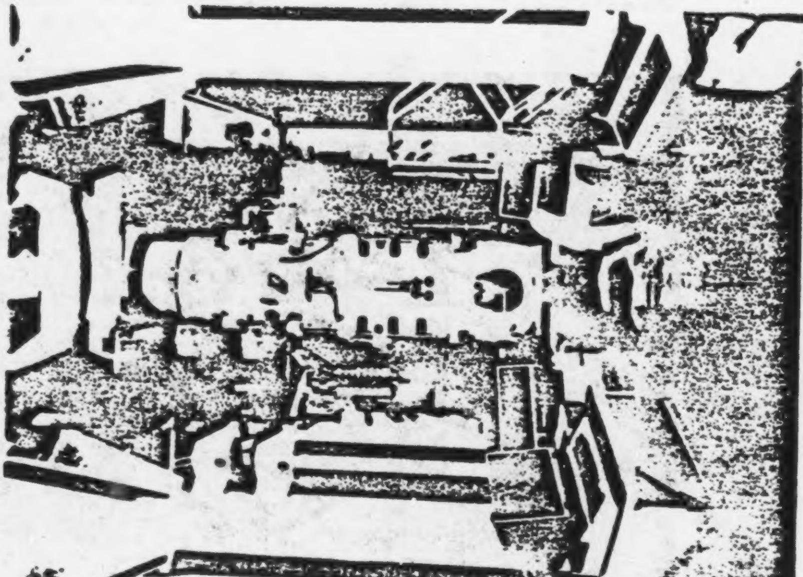
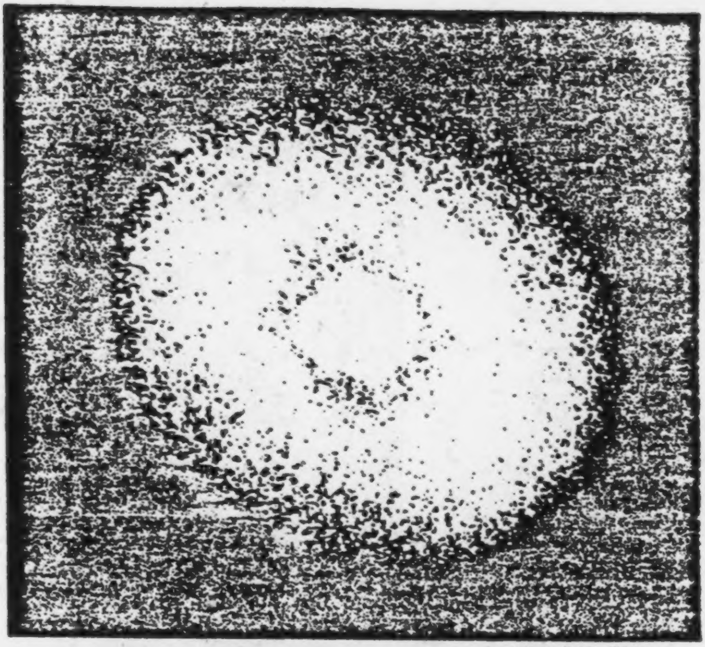


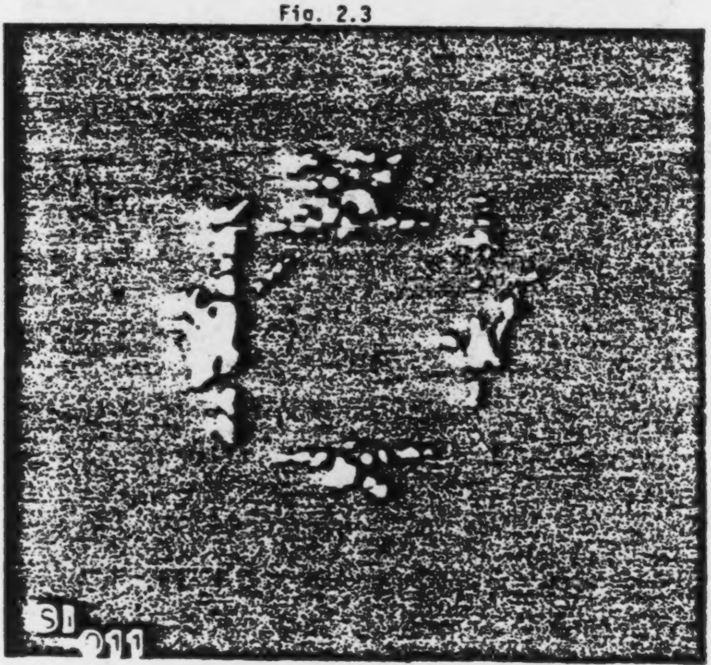
Fig. 2.1

CBB 839-8469



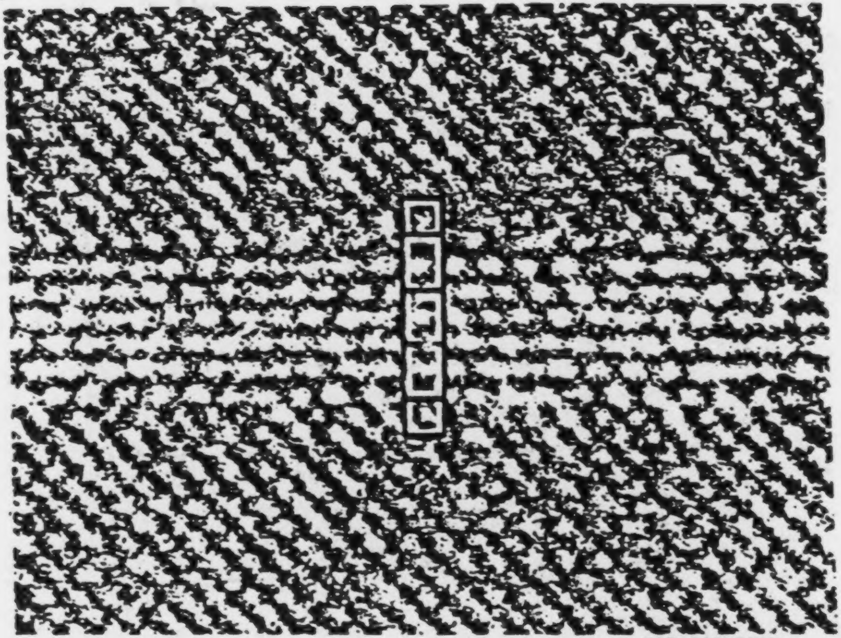
XBB 836-5044

Fig. 2.3



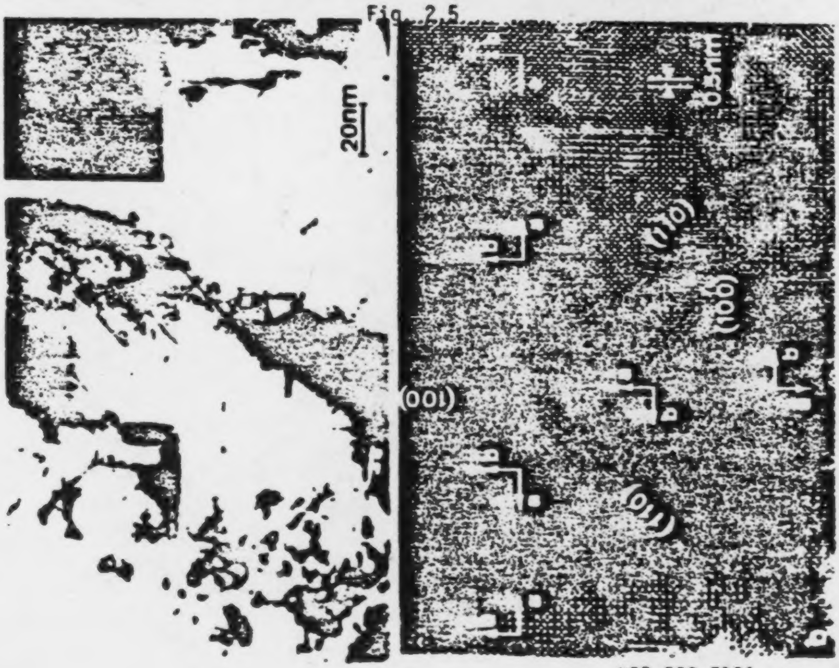
XBB 836-5042

Fig. 2.4



XBB 839-7867

Fig. 2.5


20nm
(001)
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(110)

XBB 838-7156

University of California

LAWRENCE BERKELEY LABORATORY

MATERIALS AND MOLECULAR RESEARCH DIVISION

National Center for Electron Microscopy

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The National Center for Electron Microscopy (NCEM) in the Materials and Molecular Research Division of the Lawrence Berkeley Laboratory is a high voltage electron microscope facility for ultra high resolution or dynamic in-situ studies. It is supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Science Division, U. S. Department of Energy.

(415) 486-5006; FTS 451-5006

1. THE INSTRUMENTS

1.1. Kratos EM-1500

This instrument is designed primarily for dynamic in-situ studies but it can also resolve structures at the 3A level. It is the first electron microscope to be built by Kratos with a maximum acceleration voltage of 1.5 MeV. As such, it provides accelerating voltages in the range 1200-1500kV not available elsewhere in the U.S. To achieve the higher accelerating voltage the number of stages of the Cockcroft-Walton generator was increased to 9 and the SF$_6$ insulating gas pressure was increased to ~90 p.s.i. Conditioning of the accelerator tube is carried out at 1.6 MeV. A series of 15 push buttons allows the accelerating voltage to be set at 150kV or 200-1500kV in 100kV increments. A photograph of the microscope operating level is shown in Fig. 1.

The more important instrument specifications are listed in Table I.

TABLE I: EM-1500 SPECIFICATIONS

Max$^{\underline{m}}$ Accel. Voltage		1500
High Voltage Stability		$> 5 \times 10^{-6}$/min
High Voltage Ripple		$< 3 \times 10^{-6}$
Accelerator Vacuum		10^{-7}
Obj. Lens Current Stab.		3×10^{-6}/3 min
Focal Length		6.8mm
Spher. Abb. Coeff. (Cs)		10.5mm
Chrom. Abb. Coeff. (Cc)		5.4mm
NI/E$^{1/2}$ (at 1000kV)		11
Goniometer Tilts		± 45°
Specimen Drift Rate		< 0.3Å/sec (0.5 hr.)
Vacuum	Column	$\simeq 10^{-7}$
	Spec. Chamb.	$< 3 \times 10^{-6}$
External Vibr. (pk-pk)		< 1μm
Resolution (pt-pt)		~ 3Å

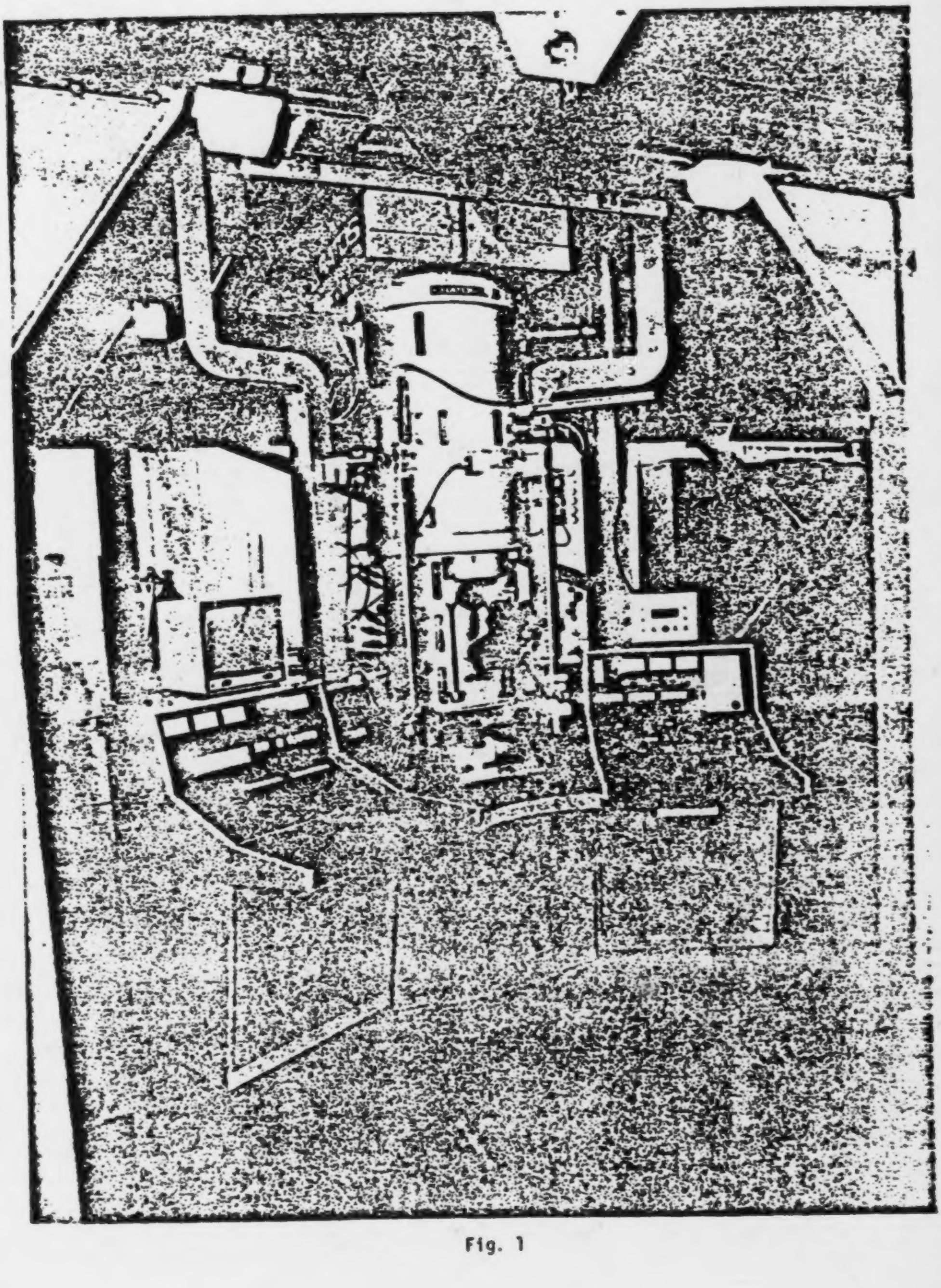

Fig. 1

The microscope is equipped with both a top-entry stage for high resolution studies, and a side-entry stage for general, dynamic in-situ, and environmental cell studies. Several different specimen stage rods are available (see Table II) and this inventory will be added to as demand develops and funding permits.

TABLE II: SPECIMEN STAGES FOR EM 1500

TYPE	X-TILT	Y-TILT	TEMPERATURE
EM 1500			
Double-tilt, cartridge-type	±45°	±45°	Ambient
Single-tilt, cartridge-type*		±45°	Ambient
Double-tilt, furnace type	±30°	±30°	Ambient-850
Single-tilt, furnace-type*		±25°	Ambient-850

*For use with Environmental Cell at pressures up to 1 atmosphere

1.2 JEOL JEM-ARM-1000

This instrument has been specifically designed for ultimate performance in the high resolution imaging mode. Attention has been given to the potential problem of specimen sensitivity to the electron beam at higher accelerating voltages however, and by incorporating a microprocessor-controlled height (Z)-variable goniometer, the microscope will operate with a constant C_s product over its entire voltage range (400kV to 1000kV). Specifications for the Atomic Resolution Microscope (ARM) at maximum voltage are given in Table III; the instrument is shown in Fig. 2.

It is also important to note that at higher lens excitation values, the microscope can be run in condenser-objective mode, enabling convergent beam electron diffraction (CBED) patterns to be taken from the same specimen areas imaged in high resolution. For increased stability, the stage configuration on this machine is top entry, employing standard 3mm diameter specimen cartridges, and coupled to a microprocessor for precise stage manipulation. The microscope uses LaB_6 filaments for additional brightness and the camera accepts 50 film cassettes.

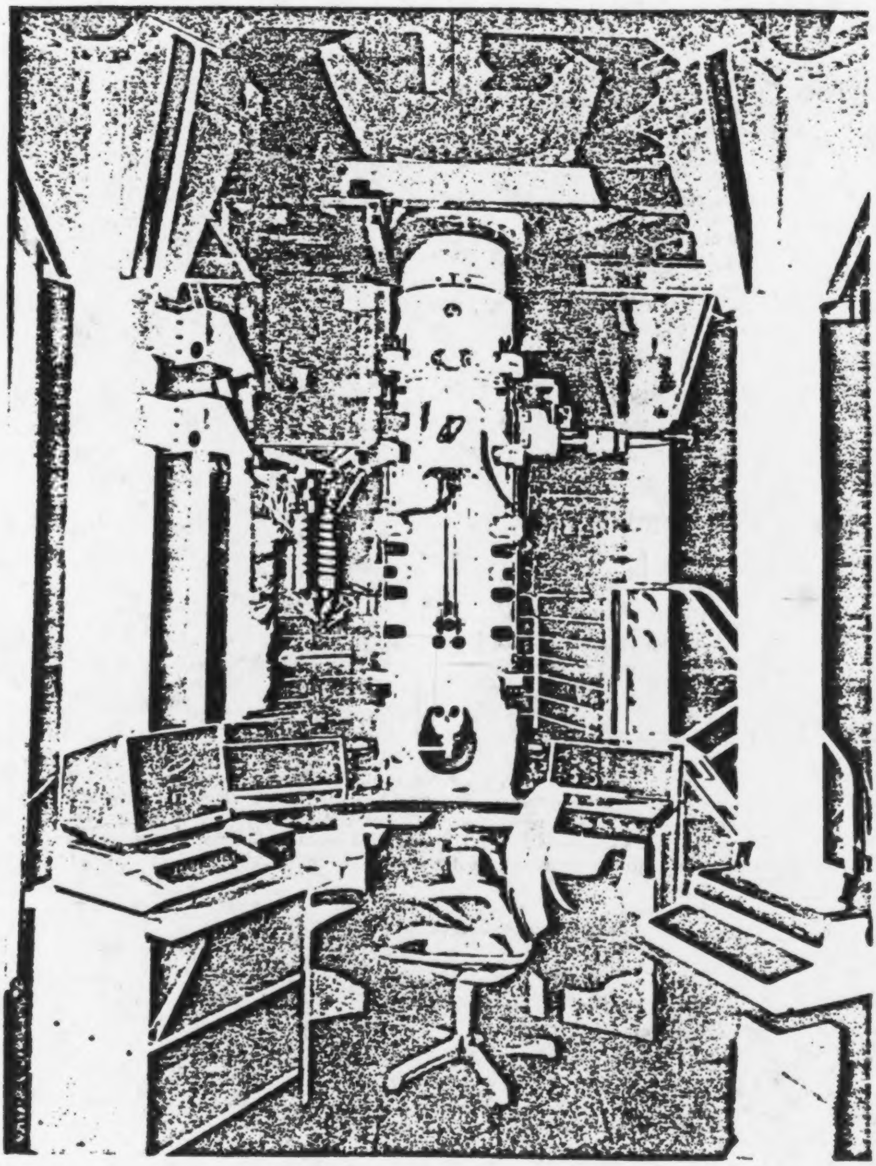

Fig. 2

Table III: JEM ARM 1000 SPECIFICATIONS

Max$^{\underline{m}}$ Accel. Voltage		1000kV
High Voltage Stability		1×10^{-6}/min
High Voltage Ripple		1×10^{-6}/min
Accelerator Vacuum		2×10^{-8}
Obj. Lens Current Stab.		1×10^{-6}/min
Focal Length		2.6mm
Spher. Abb. Coeff. (Cs)		2.8mm
Chrom. Abb. Coeff. (Cc)		3.3mm
NI/E$^{1/2}$ (at 1000kV)		23
Goniometer tilts		± 40° biaxial with lift
Specimen Drift Rate		.02Å/sec
Vacuum	Column	10^{-8}
	Spec. Chamb.	4×10^{-8}
External Vibr. (pk-pk)		< 1μm
Resolution (pt-pt)		< 1.7Å

1.3 JEOL JEM 200-CX

A support instrument to the ARM, the JEM 200-CX is well known for its high resolution performance. Relevant specifications for this machine, equipped with ultrahigh resolution goniometer (top entry), are given in Table IV. Note that specimens for this microscope must be 2.3mm in diameter in order to fit into the ultrahigh resolution pole piece.

Table IV. JEM 200-CX SPECIFICATIONS

Max$^{\underline{m}}$ Accel. Voltage		200kV
Focal Length		2mm
Spher. Abb. Coeff. (Cs)		1.1mm
Chrom. Abb. Coeff. (Cc)		1.4mm
Goniometer tilts		±10°
Specimen Drift Rate		< 0.5Å/sec
Vacuum	Column	10^{-7}
	Spec. Chamb.	10^{-7}
External Vibr. (pk-pk)		< 3μm
Resolution (pt-pt)		~2.4Å

1.4 Hitachi HU-650 (see Fig. 3)

The accelerating voltage on this instrument is continuously variable between 200 and 650kV, but it is calibrated for, and most conveniently used at three fixed voltages, 300, 500 or 650kV.

The resolution limit of this instrument is not high (see Table V) but it is adequate for some studies, exploratory experiments, and many hot stage or environmental cell experiments (see Table VI).

TABLE V: HU-650 SPECIFICATIONS

$\text{Max}^{\underline{m}}$ Accel. Voltage		650
High Voltage Stability		10^{-5}/min
High Voltage Ripple		$< 7 \times 10^{-6}$
Accelerator Vacuum		10^{-6}
Obj. Lens Current Stab.		5×10^{-5}/min
Focal Length		8.4mm
$NI/E^{1/2}$ (at 1000kV)		12.8
Goniometer Tilts		± 45°
Vacuum	Column	6×10^{-6}
	Spec. Chamb.	$\sim 10^{-5}$
Resolution (pt-pt)		~ 20Å

TABLE VI: SPECIMEN STAGES FOR HU-650

HU-650			
Double-tilt, cartridge-type	±45°	±45°	Ambient
Single-tilt, cartridge-type*		±45°	Ambient
Double-tilt, furnace-type	±30°	±30°	Ambient-850
Single-tilt, furnace-type*		±25°	Ambient-850
Single-tilt, ribbon-type*		±30°	Ambient-1000
Single-tilt, straining*		±30°	Ambient

*For use with Environmental Cell at pressures up to ~ 300 torr

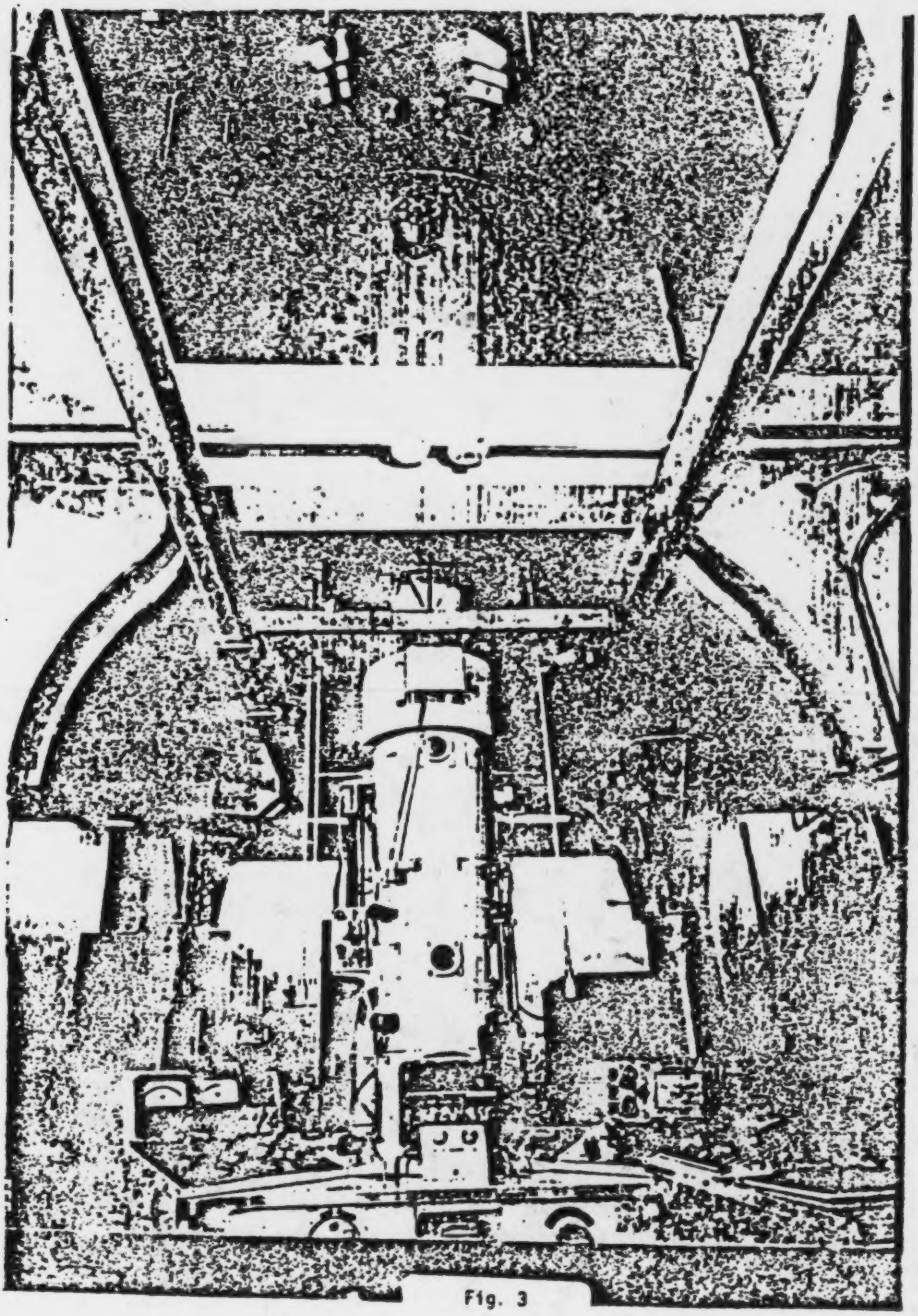

Fig. 3

2. USER POLICIES

Beam time on the HVEMs is allocated after review and acceptance of research proposals submitted in advance. The Steering Committee, composed of recognized scientists drawn from universities, industry and the national laboratories, meets at regular intervals to review, discuss, and accept project proposals and advise LBL management on Facility policies and operating procedures. The criteria used in assessing research proposals and assigning priorities are: appropriateness, scientific merit, and time availability. Proposals will remain valid for a period not to exceed 18 months. Scheduling beam time is the responsibility of the Facility Managers.

In accordance with established DOE policy, outside users must execute a Laboratory Guest Patent Agreement, an example of which is given in Appendix I.

No charges will be assessed for use of the HVEM Facility provided the proposed work is of documented programmatic interest to DOE and the results are published in the open literature. Items provided at no cost include time on the instrument, some staff assistance and advice, and use of dark rooms. Costs associated with use of effort and services outside the facility, e.g. machine shop, electronic shops, computer, stores, etc., must be borne by the user at the standard Laboratory internal rates.

If the proposed research is not of interest to DOE or is proprietary, full cost recovery (including overhead and DOE added factor) will be charged.

At the conclusion of an experimental program, regardless of the outcome, a brief report of the results and conclusions must be submitted to the Facility Managers. Copies of any publications resulting from the research must also be sent. These papers can be used to support applications for continuing or new experiments. They will also be useful as a permanent record of HVEM research activity.

Users must be qualified and experienced electron microscopists. It will be the responsibility of the Principal Investigator on the proposal to vouch for the competence of members of his team. Instructions sessions on the specific uses of the instrument will, of course, be given.

Any malfunctioning of the instruments must be reported (immediately, if serious in nature) to the Facility Support Staff or Managers. Unscheduled down-time and repairs will be minimized if all users operate the microscopes with care and consideration. Because of the disruption and inconvenience to other users, any damage to the instrument or stages resulting from operator ignorance or negligence will be repaired at the cost of the group responsible. If in doubt, seek assistance from the Facility Staff.

At least 24 hours notice is required if a microscope booking is cancelled. Failure to do so will result in loss of priority in subsequent scheduling.

3. PROPOSAL SUBMISSION AND SCHEDULING

A research proposal for using the ARM-1000 or EM-1500 should be accompanied by a Research Summary Form (RSF) (an example is shown in Appendix IV) and submitted at least 6 weeks prior to the earliest proposed starting date.

The proposal may be brief but should state clearly the scientific objective, and include use justification for the particular high voltage instrument, and a list of materials to be examined. Specimens should be prepared in advance. Any possible hazards associated with the specimens must be specified, and their possible effect on the microscope environment or specimen area must be evaluated, e.g., whether contaminating, radiation sensitive, volatile, likely to react with hot stage, etc.. Any special scheduling arrangements should be indicated on the RSF.

In the case of the ARM-1000, the proposal should be accompanied by high resolution micrographs taken on any conventional high resolution instrument together with their complete analysis and interpretation. This information will be used in assessing the need for the higher resolution or flexibility available on the ARM, and will also serve to demonstrate the operational skills of the applicants.

Experimenters may schedule time on a microscope by completing a second Schedule of Use Form (Appendix V) and return it to the Facility Administrator along with the research proposal. Non-local area users are encouraged to plan well in advance to allow local users to be assigned remaining time slots. Requests to use the environmental cell or to perform non-materials science experiments will be grouped and scheduled periodically to avoid excessive breaking of the column vacuum.

Users travelling long distances are advised to phone (415) 486-5006 for a late status report before departing.

4. SAFETY

A copy of LBL's Safety Manual will be found in the Visitors' Office and experimenters are required to familiarize themselves with the relevant portions and comply with the requirements, in addition to practicing common sense precautions in the use of equipment and facilities.

Users are also asked to sign in and out of the Facility, maintain the microscope log books, and record, for the following user's benefit, information on the working condition of the microscope. Your cooperation will be appreciated.

5. ACCOMMODATION AND TRAVEL

The responsibility for making travel and accommodation arrangements will rest with the user. However, the Facility administrative staff will be glad to give advice and assistance in making accommodation reservations when appropriate. There is a shortage of accommodation in the Berkeley area and a marked seasonal variation, so advanced reservations are highly recommended.

Appendix II lists accommodations covering a range of prices and Appendix III, information on public transportation and rental car agencies together with an area map.

(SAMPLE ONLY)

UNIVERSITY OF CALIFORNIA
LAWRENCE BERKELEY LABORATORY
PATENT AGREEMENT

This agreement is made by me with The Regents of the University of California, a corporation, hereinafter called "University", in part consideration of my employment, and of wages and or salary to be paid to me during any period of my employment, by University, and or my utilization of University research facilities.

By execution of this agreement I understand that I am not waiving any rights to a percentage of royalty payments received by University, as set forth in the University Policy Regarding Patents, hereinafter called "Policy". I further understand that I may, with the approval of the University, request a waiver determination by the U.S. Government on my identified inventions as set forth in 41 CFR 9-9.109-6, where applicable.

I agree that every possible patentable device, process, plant, or product, hereinafter referred to as "invention", which I conceive, make (first actually reduce to practice), or develop while employed by University, or during the course of my utilization of any University research facilities, shall be examined by University to determine rights and equities therein in accordance with the Policy, and I shall promptly furnish University with complete information with respect to each.

In the event any such invention shall be deemed by University to be patentable, and University desires, pursuant to determination by University as to its rights and equities therein, to seek patent protection thereon, I shall execute any documents and do all things necessary, at University's expense, to assign to University all rights, title and interest therein and to assist University in securing patent protection thereon. The scope of this provision is limited by California Labor Code section 2870, to which notice is given below, to the extent said Labor Code provision is consistent with federal law. In the event I protest the University's determination regarding any rights or interests in an invention, I agree: (a) to proceed with any University requested assignment or assistance; (b) to give the University notice of that protest no later than the execution date of any of the above-described documents or assignment; and (c) to reimburse the University for all expenses and costs it encounters in its patent application attempts, if any such protest is subsequently sustained or agreed to.

I shall do all things necessary to enable University to perform its obligations to grantors of funds for research or contracting agencies as said obligations have been undertaken by University, including the University's obligations regarding patents and technical and scientific records under Contract W-7405-ENG-48 (Contract-48) with the U.S. Government. With reference to Contract-48 I agree to abide by and fully perform the terms of Article XV of said contract, excerpts of which are set forth on the reverse side of this agreement, as they may be amended from time to time, to the extent applicable to me, and further agree that the Government shall have prior right to determine title to all such inventions, and that I will report all such inventions to the Director, Lawrence Berkeley Laboratory (LBL), or his designee. To protect the patent interests of the University and the Government, I agree not to publish any information regarding scientific or technical developments made or conceived in the course of or under Contract-48 without prior approval obtained from the Director, LBL, or his designee for this purpose.

7600-66438 (12/80)

University may relinquish to me all or a part of its right to any such invention, if, in its judgment, the criteria set forth in the Policy have been met.

I agree to be bound hereunder for and during any periods of employment by University or for any period during which I conceive, make (first actually reduce to practice), or develop any invention during the course of my utilization of any University research facilities.

In signing this agreement I understand that the law, of which notification is given below, applies to me, but that I am still required to disclose all my inventions to the University.

NOTICE

This agreement does not apply to an invention which qualifies fully under the provisions of Labor Code section 2870 of the State of California, to the extent said Labor Code provision is consistent with federal law. Said Labor Code provision provides that:

Any provision in an employment agreement which provides that an employee shall assign or offer to assign any of his or her rights in an invention to his or her employer shall not apply to an invention for which no equipment, supplies, facility, or trade secret information of the employer was used and which was developed entirely on the employee's own time, and (a) which does not relate (1) to the business of the employer, or (2) to the employer's actual or demonstrably anticipated research or development, or (b) which does not result from any work performed by the employee for the employer. Any provision which purports to apply to such an invention is to that extent against the public policy of this state and is to that extent void and unenforceable.

In any suit or action arising under this law, the burden of proof shall be on the individual claiming the benefits of its provisions.

*Employee/Guest Name ________________________________
(Please Print)

Employee/Guest Signature ______________________ Date: ______________

Witness Signature: ______________________ Date: ______________

Excerpts from Modification No. 23
Contract No. W-7405-ENG-48

(b) *Allocation of principal rights.* (1) Assignment to the Government. The University agrees to assign the Government the entire right, title, and interest throughout the world in and to each Subject Invention, except to the extent that rights are retained by the University under paragraphs (b) (2) and (c) of this clause.

(e) *Invention identification disclosures and reports.* (1) The University shall establish and maintain active and effective procedures to ensure that Subject Inventions are promptly identified and timely disclosed. These procedures shall include the maintenance of laboratory notebooks or equivalent records and any other records that are reasonably necessary to document the conception and/or the first actual reduction to practice of Subject Inventions, and records which show that the procedures for identifying and disclosing the inventions are followed.

(f) *Publications.* It is recognized that during the course of the work under this contract, the University or its employees may from time to time desire to release or publish information regarding scientific or technical developments made or conceived in the course of or under this contract. In order that public disclosure of such information will not adversely affect the patent interests of DOE or the University, patent approval for release or publication shall be secured from Patent Counsel prior to any such release or publication.

NOTE

At LBL, patent related duties and functions have been delegated by the Director to the LBL Patent Group. Employees are therefore requested to contact the LBL Patent Group for processing of patent matters.

Revised December 1, 1980

Appendix IV
Proposal ________
(assigned by NCEM)

National Center for Electron Microscopy, Berkeley
Research Summary Form

MMRD, Bldg. 72
University of California
Lawrence Berkeley Laboratory
Berkeley, CA 94720
(415) 486-5006

Title of Project:

P.I./Reseacher	Address	Phone Numbers Office	Phone Numbers Home	Please check appropriate box		
				☐	☐	☐
				☐	☐	☐
				☐	☐	☐
				☐	☐	☐

Request to operate microscope
Request instruction to operate microscope
Will not operate microscope

Source and duration of project funding:

Estimate of Facility time required (no. of 8-hr. shifts)________________

Preferred HVEM* ARM 1000 / EM 1500 / HU 650

1st Preference________________
2nd Preference________________

Scheduling Requirements:
Earliest possible starting date:________________
Latest possible starting date________________
Other time requirements:________________
Anticipated completion date:________________

Special Equipment Requirements (e.g. stages, environmental cell, gases, etc.):

*Although the 1st preference will usually be obvious, please check 2nd preference and also indicate if preliminary work can be carried out on the HU 650.

NOTE: We, the investigators named above, have read, have understood and will comply with the operational requirements of the Facility as set forth in the Users' Guide.

Signature________________ Date________________

6.0 Los Alamos National Laboratory

6.1 Spallation Neutron Research/Proton Storage Ring (SNR/PSR) Facility

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

Answer: The SNR/PSR facility can provide the condensed matter science community with world class capabilities in the new domain of energy and momentum transfer provided by the very high epithermal neutron flux. The high peak thermal flux, combined with the time of flight (TOF) method, offers experimental capabilities in the thermal range that can compete favorably with most steady-state reactors in the world. In addition, the use of the TOF technique at the SNR/PSR pulsed source offers many characteristics that are complementary to steady-state sources.

There are many areas of condensed matter science where an advanced pulsed source, such as the SNR/PSR, is advantageous compared to other methods.

PHASE TRANSITION PHENOMENA - These can be studied by using TOF methods to cover a large range in momentum and energy transfer simultaneously. For example, diffuse scattering can see domain formation, superlattices, amorphous structures, and critical scattering in planes or rods. Inelastic scattering with TOF methods can be used to conduct surveys of unknown dispersion curves of elementary excitations. TOF methods are particularly useful in the study of phase transitions induced by high pressures, electric fields, or magnetic fields.

HIGH ENERGY EXCITATIONS - The momentum distributions n(p) of quantum solids and fluids (e.g., the Bose condensate in He-II) can be studied by recoil scattering with epithermal neutrons in the impulse approximation limit. The SNR/PSR may play an essential role in unraveling the mysteries of itinerant magnetism through the measurement of high-energy ($50 < \hbar\omega < 500$ meV) magnetic excitations such as spin waves and Stoner excitations. It should also be possible to measure presently inaccessible high-energy phonons in materials such as metal hydrides, graphite intercalates, etc. Pulsed sources are already established as the method of choice of high-energy chemical spectroscopy with neutrons.

STRUCTURAL STUDIES - The study of the structure of liquids and amorphous materials is particularly well suited to the SNR-PSR because one can use the high epithermal flux to scatter at large values of Q to get excellent real-space resolution and because the inelastic contributions to the scattering are minimized. The SNR/PSR will play a significant role in the study of low-dimensional materials, because TOF methods permit one to readily integrate over irrelevant dimensions. Pulsed sources, such as the SNR/PSR, are already established as the preferred method for powder diffraction because of the constant resolution function, small d spacings, and high data rates that can be achieved and because of the advanced state of the Rietveld powder profile refinement data analysis method. They may also be revolutionary for single-crystal diffraction, in part because of the ability of TOF methods to measure twinned or multiple crystals or domains and in part because the high data rates of TOF methods may permit the use of very small crystals. These high data rates enormously simplify sample preparation requirements.

SPECIAL SAMPLE CONDITIONS - TOF methods are clearly preferred for experiments requiring limited sample access, such as high pressures, or the application of electric or magnetic fields. They are clearly advantageous for pulsed sample environments where the external stress cannot be maintained (e.g., the high intensity laser excitation of a biological sample).

There are other areas of enormous current interest in condensed matter science where the potential of the SNR/PSR needs to be explored.

BIOLOGY, POLYMERS, AND METALLURGY - Cold neutrons are essential to the application of neutron scattering in these areas because of the large scale of the structures of interest. A National Academy of Sciences Committee identified small angle neutron scattering and quasielastic scattering at 10-microvolt resolution as areas in which an urgent U.S. effort should be generated to catch up with Europe. Estimates of instrument performance from the Spallation Neutron Source in the U.K. indicate that the SNR/PSR with 200 microamperes and an optimized 20 K cold H_2 source could come within a factor of two of ILL performance in these areas. In addition, these instruments will have an order of magnitude larger dynamic range than their reactor equivalents. SANS on a pulsed source will automatically provide discrimination against inelastic scattering and have superior q resolution to permit low resolution crystallographic studies of macromolecules. The pulsed source equivalent of neutron spin echo with a larger range would be particularly valuable in the study of relaxation phenomena.

POLARIZED NEUTRONS AND MAGNETISM - Full use of polarized neutrons at a pulsed source is essential for its application to magnetism. Spin modulation techniques may be required to obtain high resolution for high-energy neutrons. At short wavelengths, this will require the development of efficient methods for white beam polarization. In the longer wavelength region, supermirror technology can be readily adapted to the SNR/PSR facility. Methods for the study of high-energy magnetic and electronic excitations need further development. They require scattering with high-energy neutrons at low q, which introduces problems of available phase space and multiple scattering. However, it is clear that pulsed sources are kinematically favored over reactors for these studies.

DYNAMIC STUDIES - The study of time-dependent phenomena such as the response of a polymer to an applied stress, needs to be fully explored with SANS methods.

The TOF method produces high data rates and large amounts of data, which has usually been regarded as a problem because of computer limitations and the lack of physical interpretation during the course of an experiment. However, with modern computer technology it is now practical to handle these data rates and to process it on line to display the results in physical terms using high-quality graphics.

There is no single number by which one can compare the performance of a pulsed source to a reactor. Direct comparison can only be carried out on an experiment-by-experiment basis. However, it has already been demonstrated that even the weak pulsed sources currently available are already superior to the best reactors for powder diffraction, liquids and amorphous materials diffraction, and vibrational spectroscopy of molecules. At the same time, there is no concept for a pulsed source instrument that will be as flexible as a triple-axis spectrometer at a reactor for the measurement of elementary excitations. A healthy U.S. neutron scattering program will use pulsed sources and steady state sources in complementary ways.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

Answer: The SNR/PSR will be a unique pulsed facility when the PSR becomes fully operational in 1986. The SNR/PSR will operate at 12 Hz, 100 microamperes of 800 MeV protons, with a 270 nsec pulse width. The peak thermal neutron flux of the SNR/PSR in 1986 will be 1.7×10^{16} n/cm^2-sec, which will be the highest in the world, more than an order of magnitude better than the best research reactors and almost two orders of magnitude more than present pulsed source capability in the U.S. This peak flux is a factor of 2 higher than the Spallation Neutron Source under construction in the U.K. and scheduled for operation in late 1984.

The peak thermal flux could be as high as 5×10^{16} n/cm^2-sec. The SNR/PSR will also produce a much higher epithermal ($E > 100$ MeV) neutron flux (four orders of magnitude higher at 1 eV than existing reactor neutron sources) to open a new energy and momentum transfer domain for neutron scattering. The low repetition rate of 12 Hz will give the SNR/PSR the largest dynamic wavelength range of any pulsed source in the world.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

Answer: There are presently three neutron scattering instruments in the national user program at the SNR/PSR facility. These include:

Be - BeO FILTER DIFFERENCE SPECTROMETER - Inelastic scattering experiments in chemical spectroscopy, dispersionless modes, and phonon density of states. $30\ \text{meV} < \hbar\omega < 1000\ \text{eV}$ with approximately 5% energy resolution.

SINGLE CRYSTAL DIFFRACTOMETER - Single crystal diffraction by the Laue-TOF method with up to 30 Angstrom unit cell axis. Also suitable for structural studies of multiple crystals or domains, diffuse scattering, high pressure diffraction, because of the large range in reciprocal space covered by a single histogram in the time-of-flight method. Variable temperature ($10\ \text{K} < T < 300\ \text{K}$) and variable resolution capability.

NEUTRON POWDER DIFFRACTOMETER - Moderate resolution (~ .45%) diffraction experiments on powder samples, to be analyzed by the Rietveld powder profile refinement technique by backscattering at 150 degrees. Also 90 degree detector bank for special environment experiments, and a low angle 14 degrees detector bank for liquids and magnetic materials diffraction.

There are currently three prototype instruments in operation at the SNR/PSR to gain experience toward the eventual construction of well-engineered instruments for the national user program. These are:

LIQUIDS, AMORPHOUS, AND SPECIAL ENVIRONMENT DIFFRACTOMETER - Low resolution, high intensity diffraction (~1-2%) at low angles (5, 14, 40, 90, and 150 degree detector banks) for liquids and amorphous materials diffraction minimizing inelastic scattering (Placzek) contributions. Also optimized for high pressure, high and low temperature, special sample cell powder diffraction.

ELECTRON VOLT SPECTROMETER - Inelastic scattering experiments at low Q to see magnetic and electronic excitations by the use of nuclear resonance filter difference methods. Built in collaboration with the Rutherford-Appleton Laboratory. Uses a novel arrangement of in-beam coarse filters to minimize statistics errors due to the use of a difference technique. Presently using Sm filters.

CONSTANT Q SPECTROMETER - Inelastic neutron scattering experiments on elementary excitations in single crystal samples (such as phonons and magnons). Large range in Q, space covered simultaneously in the TOF method (depending on choice of analyzer crystal plane for analysis). Characteristics complementary to triple axis spectrometers at reactors. Capable of a simultaneous constant vector Q scan through data manipulation.

Other spectrometers are under development, although not yet operational, at the SNR/PSR. These include a chopper spectrometer and a small angle diffractometer.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer: Research highlights from 1981 to the present include both novel scientific results and the development of new TOF neutron scattering instrumentation. The scientific highlights include:

- Discovery of the first organometallic complex that reversibly binds molecular hydrogen.
- High pressure structure of ReO_3 by single crystal neutron diffraction.
- Model independent determination of the hydrogen-hydrogen pair correlation function in liquid water, showing a more ice-like structure than molecular dynamics simulations.
- Systematic study of the correlation of vibrational frequency with bond length of short intramolecular hydrogen bonds.
- Determination of the anharmonic force constants of metal hydrides through the use of high energy inelastic scattering.
- High energy transfer vibrational spectra of chemisorbed hydrogen on Raney and coprecipitated nickel, leading to identification of bonding sites.
- Determination of the momentum distributions of atoms in solids by recoil scattering at high Q, the impulse approximation limit.

Instrumentation development highlights include:

- First Be-BeO filter difference spectrometer for high data rate vibrational spectroscopy.
- Development of the nuclear resonance filter difference method for electron volt spectroscopy.

- Development of a method for high pressure single crystal diffraction by the TOF technique.
- Demonstration of the ability to study multiple crystals or domains by TOF single crystal diffraction.
- Development of a high data rate (400 nsec) Anger Camera for position sensitive neutron detection.
- Development of a high speed (36,000 rpm) magnetic bearing neutron chopper and phasing to mains.
- New two axis goniometer for single crystal diffraction.
- Constant Q Spectrometer development, and observation of phonon dispersion by the TOF method.
- Many benchmark target/moderator/reflector experiments.

Anticipated progress in FY 84 and FY 85 - Generally it is extremely difficult to accurately predict scientific progress, although we expect it to be along the directions of the answers to question 1. Some areas where progress can confidently be predicted are:

- Further demonstration of TOF diffuse scattering methods on the single crystal diffractometer to study phase transition phenomena, including superlattices, domain formation, and critical scattering.
- High pressure structures of Hydrogen and Deuterium.
- Application of the constant Q spectrometer to the study of high energy magnetic excitations in itinerant magnet systems.
- Operation of well-engineered versions of the above developmental instruments, bringing them into the national user program and opening up several new areas of neutron scattering research.
- Strong application of scintillator detector technology to TOF neutron scattering instrumentation, permitting much larger solid angles, dynamic ranges, and data rates.

5. What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?

Answer: The most important facility change will be the operation of the Proton Storage Ring bringing the world's highest peak neutron flux to make the SNR/PSR the premier pulsed spallation neutron source in the world. At 100 microamperes, 12 Hz, and 270 nanosecond proton pulse width on a depleted uranium target the combined SNR and PSR facility will have 60 times the current time average intensity, 600 times the current peak intensity, ten times the wavelength dynamic range, and up to 25 times the TOF resolution of the current SNR facility. This will provide the U.S. with world class neutron scattering capability.

Other facility changes in FY 81 to present include the construction of a laboratory support building (3200 sq. ft.), a warehouse (1800 sq. ft.), and the upgrade of the SNR beam transport system and target area to handle 100 microamperes.

There has been a continual improvement in neutron output and the number of simultaneous experiments which can be operated, as follows:

1981 - Operation of a lightly moderated tantalum spallation target producing 10 neutrons/proton.

1982 - Operation with a lightly moderated tungsten spallation target producing 13 neutrons/proton.

1983 - Installation of a highly reflected moderating system with a tungsten target capable of serving 6 experiments simultaneously.

1985 - Installation of a fully reflected self shielding moderating system with a cryogenic temperature surface, depleted uranium target producing 26 neutrons/proton and the capability of serving 15 experiments simultaneously.

As the neutron scattering research program at the SNR/PSR is new, and only began a significant growth after 1981, the additional facility change has been the steady build up of neutron scattering instrumentation.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer:

NEUTRON SCATTERING RESEARCH (In House/National User Program)
B/A In Thousands

	Ofc. of Basic Energy Sciences Div. of Materials Sciences	Other*
FY 81	$ 819	$ 600
FY 82	1190	635
FY 83	1530	710
FY 84	1570	800
FY 85	1800	1165

*Other refers to other LANL programs.

OPERATIONS (All SNR operations including defense programs (OMA), nuclear science, and materials science)

(B/A in Thousands)

	Ofc. of Basic Energy Sciences Division of Materials Sciences	Other
FY 81	$ 0	$1373
FY 82	0	1578
FY 83	0	1450
FY 84	0	1600
FY 85	500	(1700)
CAPITAL		
FY 81	130	13
FY 82	250	50
FY 83	250	50
FY 84	300	90
FY 85	600	100
CONSTRUCTION		
FY 81	0	390 (GPP)
FY 82	0	0
FY 83	2700	0
FY 84	0	0
FY 85	0	0

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer: None has been provided or expected from any of these sources.

8. **For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.**

Answer:

Neutron Scattering Research and Operations

	Staff Member (FTE)	Technical Support (FTE)
FY 1981	13.3	14.5
FY 1982	17.0	15.0
FY 1983	16.0	14.0
FY 1984	19.4	17.3
FY 1985	22*	19.5*

An FTE is equivalent to one full time employee working 2,080 hours.

* Estimated

9. What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?

Answer: The SNR/PSR research program obtained its first scientific results in 1981, with a largely in-house research program. A formal national user program at the SNR/PSR facility began in 1983 with two instruments, expanding to three instruments, and is projected to reach six instruments in 1985. At the same time, two to three instruments are in a prototype development stage prior to eventual entry into the formal user program. Based on present experience and expressions of interest from users, there is no question that the SNR/PSR facility will have heavy pressure on available beam time. We expect approximately 10 instruments to be in operation by 1987 with approximately 200 experimenters using the facility. In terms of efficiency of operation, the SNR has been available for 96% of available LAMPF beam time from 1981 to 1983. The SNR operated for 2,140 hours in FY 1984 for six beam lines in place.

10. For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?

Answer: Since the formal national user program began in 1983, there have been 39 Program Advisory Committee approved proposals for experiments at the SNR facility using the first three user instruments. These were conducted in 1983 or will be conducted in 1984. In addition, there have been approximately 50 experiments conducted on Laboratory discretionary time or before the instruments were ready for entry into the formal user program. We would project approximately 50 experiments to be conducted as part of the formal user program in 1985.

11. What is this facility's user policy?

Answer: The SNR/PSR is being developed as a national user facility for neutron scattering research. A formal proposal procedure has been developed for the use of neutron scattering instrumentation, with a nationally appointed Program Advisory Committee (PAC) in cooperation with the Argonne National Laboratory to review proposals. The PAC is expected to make its recommendations on the basis of scientific excellence and optimal use of SNR/PSR characteristics. The PAC allocates two-thirds of the available neutron scattering beam time at the SNR/PSR. One third of the beam time is reserved for Laboratory discretionary research, defense programs, and instrument development. The use of neutron scattering instrumentation is free of charge to outside experimenters with approved proposals. Laboratory, university, and industrial proposals are treated on an equal basis. Following DOE policy, proprietary experiments will be conducted on a full cost recovery basis.

12. For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?

Answer: None has taken place.

13. What is the mechanism by which specific research proposals for experiments at the facility are considered?

Answer: Formal proposals are reviewed by a nationally appointed Program Advisory Committee twice a year. At present, the PAC is shared with the IPNS program at Argonne National Laboratory. Further details can be found in the answer to question 11.

14. How many research proposals have been submitted over the past five years, and how many of these have been approved?

Answer: The formal national user program at the SNR facility only began in 1983 with two instruments. To date, 55 proposals have been submitted, and 39 have been approved. However, requests for beam time have exceeded by more than three times the amount available. The PAC has generally reduced the beam time requests on approved experiments.

15. How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?

Answer: Of PAC-approved experiments, 11 faculty personnel have been users to date. There have been approximately 15 additional university personnel who have used the SNR facility outside of the formal user program, making a total of 26.

16. How many industrial researchers have utilized the facility over the past five years?

Answer: Two industrial researchers have been users to date.

17. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer: Of PAC-approved experiments, there have been 10 foreign users of the SNR/PSR facility. There have been an approximately equal number of foreign visitors who have utilized the facility outside of the formal user program.

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: Of PAC-approved experiments, there have been 20 experimenters from other (non-LANL) federally sponsored laboratories. There have been approximately 30 such users outside of the formal user program.

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: There are many potential future development possibilities for the existing Spallation Neutron Research/Proton Storage Ring (SNR/PNR) Facility, but there are no specific plans to undertake any of them beyond the construction activities identified in the FY 1985 budget request.

20. Please provide a copy of the facility's latest annual report.

Answer: There has been no annual report prepared for this facility. However, relevant excerpts from the 1983 "Progress at LAMPF" report follow.

IV. PROTON STORAGE RING CONSTRUCTION AND RESEARCH PROGRAM DEVELOPMENT

Overview

C. D. Bowman

A world-class facility is under development on Line D for pulsed neutron and other research. The principal elements in this facility are the Proton Storage Ring (PSR) now under construction and the existing Weapons Neutron Research (WNR) facility target and experimental areas. The storage ring will convert the long LAMPF macropulses into short, intense proton bursts for a variety of experimental programs. Two pulse structures will be provided: the long-burst, low-frequency (LBLF) mode with 270-ns pulses at 12 Hz for an average current of 100 μA, and the short-burst, high-frequency (SBHF) mode with 1-ns pulses at 720 Hz for an average current of 12 μA.

The long-burst mode will be devoted primarily to condensed matter research using pulsed neutron scattering techniques and will be the major facility for this type of pulsed neutron research in the United States. A User program is being developed under the auspices of the Division of Materials Science of the USDOE, which should grow to more than 100 Users annually when the PSR becomes operational. This User program began in calendar year 1983 with the availability of pulsed neutrons produced by 5-μs bursts of LAMPF beam on the present WNR target-moderator system. More than 100 visitors from 30 institutions participated in the pulsed-neutron planning and research in 1983.

Plans also were completed for a major increase in experimental space around the WNR target area to accommodate as many as 15 spectrometers for this research. Funds were received in FY 1983 for a $2.7-million 3-year WNR program to upgrade the target area and beam-transport system to handle the required current and to improve the neutron-production target and shielding.

Research in the field of neutron-nuclear physics will receive a major boost from the short, intense bursts of neutrons produced from the PSR, the extension of useful neutron energies up to several hundred MeV, and the absence of an intense gamma flash associated with the neutron burst. Neutron physics experiments were performed this year at the WNR using sub-micro-amp currents of LAMPF micropulses. Although these experiments are unsurpassed in intensity and resolution, orders-of-magnitude improvements will be possible when the PSR short-pulse mode becomes operational.

The low duty cycle and high-current capacity of the PSR almost certainly will be major advantages for low-energy neutrino research. In anticipation of such a program, a new beam line (Line E) has been assembled parallel to Line D and in the Line D channel, with a pulsed magnet for multiplexing LAMPF beam between Lines D and E. Neutrino experiments requiring an unshared target will be conducted on this line using a target and detector area now under construction.

The rapid progress on the installation of Line E, carried out by a collaboration of Los Alamos Groups P-3, P-9, P-14, and MP Division, the University of New Mexico, University of California at Riverside, and Temple and Valparaiso Universities, should enable measurements on ν_μ-nucleus charged-current cross sections during the summer of 1984. These data are crucial for the design of future detectors for use with any Los Alamos neutrino source. This measurement also will provide data on possible $\nu_\mu \rightarrow \nu_e$ oscillations with a sensitivity of about 10^{-3}, although this is far from the limit ultimately achievable at LAMPF.

The construction of the PSR is supported by Laboratory Defense Program Funding. A substantial defense research program will be conducted using the PSR and associated facilities. On infrequent occasions, defense

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The WNR/PSR facility, located south [illegible] PF switchyard, accepts 800-MeV proton [illegible] the LAMPF accelerator. Its design was accomp[illegible] by the Accelerator Technology (AT) Division of L[illegible] National Laboratory.

The research program at WNR/P[illegible] is [illegible] by the Physics (P) Division at Los Alamos and is supp[illegible]ly by Laboratory internal funding and the Office of Energy Research of the USDOE. Researchers from P Division collaborate with other Los Alamos staff and outside Users in their experiments.

Progress at LAMPF **thanks the management of P Division, especially Charles Bowman, for this section of reports on developments and research at WNR/PSR.**

programs will require the unshared use of the PSR, but the typical defense experiment will only require the use of one or more of the many neutron drift tubes that view a common pulsed source of neutrons.

Participation in the PSR research programs is encouraged. Interested individuals should contact Richard N. Silver for condensed matter physics, and Gerard J. Stephenson for neutron or neutrino physics.

PSR Construction

G. A. Sawyer

The PSR is a major addition to the WNR facility at LAMPF. It will be a bunch compressor for the relatively long linac macropulses from LAMPF, tailoring them into short, intense pulses ideally suited for neutron-scattering research.

The PSR is located in a tunnel adjacent to, and below the level of, the existing beam line (Line D) that serves the WNR facility. A plan view of the ring and tunnel, showing component locations, is given in Fig. 1. Beam enters the ring from Line D; after accumulation, it returns to Line D, through which it is transported to the WNR neutron-production target. Connections with Line D are made by short, sloped, beam-transport channels. Located above the ring tunnel and on top of a 4.9-m-thick earth shield are service and assembly buildings.

The ring operates in two accumulation modes, each independently optimized to provide the desired neutron-source pulse structure for nuclear physics and materials research programs.

Operational characteristics of the two PSR storage modes are summarized in Table I. In the short-bunch high-frequency (SBHF) mode, protons are accumulated in six equally spaced 1-ns bunches during each LAMPF macropulse. The bunches are individually extracted by a fast kicker during the 8.2-ms interval between injection pulses. Because the linac macropulse frequency is 120 Hz, this program produces an extraction rate of 720 pps. For PSR injection, the final 108 µs of each macropulse is modified by a chopper-buncher system in the linac low-energy transport to form a sequence of micropulses spaced at 60-ns intervals. The ring circulation period is chosen so that this injected pulse train is synchronized with the six bunches already stored. Each incoming micropulse, containing 3.3×10^8 protons, merges with a ring bunch; 300 micropulses are accumulated in each ring bunch. The narrow bunch width in this mode is maintained by a high-frequency buncher located in the ring.

In the long-bunch low-frequency (LBLF) mode, the ring accumulates complete linac macropulses (5.2×10^{13} protons) in a single 270-ns bunch. Each stored bunch is extracted after completion of the injection cycle, with a maximum delay of 4 ms. The cycle repetition rate is 12 Hz. Peak current, assuming a parabolic longitudinal charge distribution, is 46.3 A; average circulating current is 100 µA. For injection, a slow-wave chopper in the linac low-energy transport carves 90 ns out of each 360 ns throughout the macropulse, permitting entering pulses to be overlapped with those that are already stored in the 360-ns circulation period. A first-harmonic buncher keeps the 90-ns gap clear of protons to facilitate low-loss

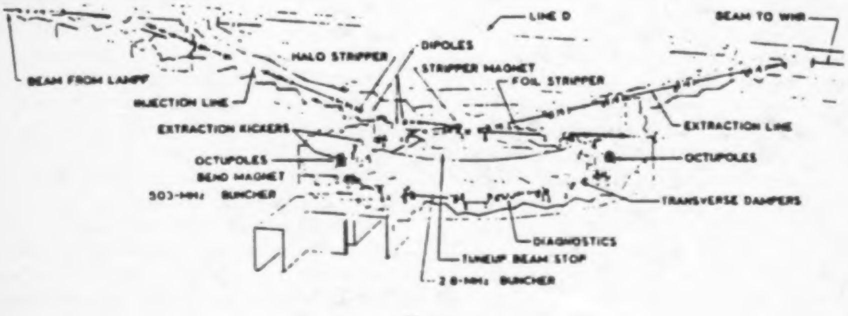

Fig. 1.
Plan view of the Proton Storage Ring.

Table I. PSR Operating-Mode Characteristics.

	Short Bunch, High Frequency	Long Bunch, Low Frequency
Parameter	Nuclear physics	Materials science
Number of bunches in ring	6	1
Bunch length in ring	1 ns	270 ns
Bunch interval in ring	59.63 ns	—
Buncher frequency	603.75 MHz	2.795 MHz
Protons/bunch accumulated	1×10^{11}	5.2×10^{13}
Accumulated turns	300	2100
Injection rate	120 bursts/s	12 pps
Filling time	108 μs	750 μs
Extraction rate	720 pps	12 pps
Peak circulating current	24.0 μA	100 μA

extraction. After accumulation is complete, the ring is emptied in a single turn by the fast-extraction kicker.

The PSR was authorized as a $21.8-million construction project in FY 1981, and a staging building for development and assembly of equipment was built by the end of that year. Construction of the main-ring tunnel and its associated equipment building started in May 1982 and is now complete.

It was necessary to develop specialized equipment systems for the PSR, including an intense negative-ion source, a beam chopper to provide the desired beam-bunch pattern, kicker magnets to deflect the beam into and out of the ring, and beam bunchers to compress the beam into well-defined short pulses. These developments have been under way for several years and satisfactory designs are proven for all systems. Final component assembly is in progress.

Procurement of standard equipment, such as magnets and vacuum components, is nearly complete and installation in the ring has started.

First operation of the PSR is expected on schedule in the spring of 1985. At first the beam current will be small, but as tuneup proceeds, the beam current will increase and we expect to reach the 100-μA level at the end of FY 1986.

WNR Upgrade

R. Woods

The WNR upgrade will raise beam-handling capability to the 100-μA level of the PSR design. The project requires improvements to the proton beam-transport line and the target-moderator-reflector (TMR) system.

To allow continuing hands-on maintenance of the proton beam-transport line under higher current conditions, beam losses must be kept low, requiring a larger aperture in the beam-transport system. The change from H^+ to H^- and the revamping of the switchyard also require reworking the beginning of Line D. There are time-sharing modes in which some beam will be going to the PSR and other beam pulses will be going either to the WNR or to the neutrino facility. A kicker magnet and stripper foil will be mounted in Line D to permit this time sharing.

The major thrust of the upgrade will be seen in the TMR. The increased current, from 10 to 100 μA, must be dissipated in the new design. We are also planning for a depleted uranium target and designing to permit the installation of a boosted target in the future.

The new concept for the TMR is shown in Fig. 2. The concept is a split target with a void between and moderators located around this void in an arrangement termed the flux trap geometry. The neutron flight paths that view these moderators thus will not "see" the neutron target itself. This arrangement significantly reduces the background of unwanted high-energy neutrons.

The existing WNR flight paths will view these moderators. The upper target will be provided with wing moderators that can be viewed by future flight paths. In this design the target and moderators are surrounded by a 1-mm-diam cylinder of material that reflects neutrons back into the moderators and also adds to the shielding.

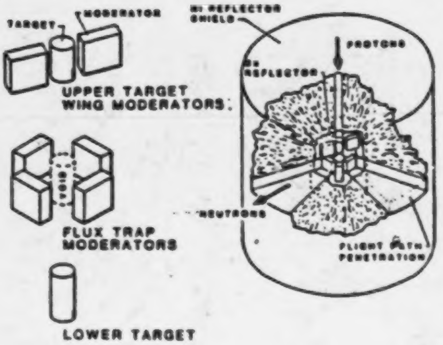

Fig. 2.
New concept for target-moderator-reflector (TMR) system.

The installation of a depleted uranium target in the spring of 1985 will give a factor of ~2 in useful neutron production. A liquid-hydrogen moderator also will be installed at that time to provide a source of cold and ultracold neutrons. A separate insertable target with little or no moderation will be provided for higher energy neutron experiments.

The increased neutron flux resulting from these improvements requires an additional 0.6 m of iron shielding above the WNR target for equipment protection; additional shielding and a water-cooled beam stop also will be provided below the WNR target.

Experimental Halls Expansion

H. Robinson

The original plan for the existing WNR experimental hall did not contemplate the 100-fold increase in neutron source capability made possible by the PSR. This greater intensity and optimized pulse structure from the PSR transforms the source into the most intense spallation neutron source in the nation, and perhaps in the world. These extraordinary capabilities have proved attractive not only to the Los Alamos National Laboratory staff, but to a large contingent of researchers from universities and industry. Soon after the PSR becomes operational, the facility expects to host approximately 100 visiting experimenters each year.

To provide an adequate experimental area to accommodate the User community and permit the full use of the neutron source, construction funding of $15.7 million is requested for FY 1985 to expand the present experimental hall and support facility.

This funding will provide a 929-m^2, pre-engineered, high-bay structure attached to the east side of the existing hall on the existing grade. The hall will be equipped with the full complement of services required for six major neutron-scattering spectrometers. A 186-m^2 pre-engineered wing attached to this structure, shown in Fig. 3, will house quiet rooms, set-up areas, and restroom facilities.

In addition, a 1115-m^2 reinforced concrete subterranean structure attached to the west side of the existing hall at the same floor elevation will be built. The complement of mechanical and electrical services provided in the east hall will be installed here for six more experiments.

A 745-m^2, two-story, reinforced concrete and pre-engineered laboratory and support complex will adjoin the present control room and the west experimental hall. This building, shown in Fig. 4, will be equipped for offices and used for data collection and technician work space.

Modifications will be made to the existing hall to allow better access and control of experiments and to provide penetrations for additional neutron-beam tubes from the target crypt. The proposed project includes funding for the construction of three new spectrometers especially designed to make optimum use of the intense pulsed-neutron beam, plus funding for six additional data-collection computers and a hub computer for data analysis.

In summary, the combined floor space of the experimental halls (2230 m^2) will more than quadruple the space available for the spectrometers and staging of experiments, thus assuring full use of the source for the national neutron-scattering program. The 743 m^2 of support area on the west side will provide adequate room for data collection and light technician service to experimenters using this world-class facility.

Line E for Neutrino Physics

T. Dombeck and G. J. Stephenson, Jr.

The neutrino beam line designated Line E lies to the south of the LAMPF switchyard in the WNR complex, as shown schematically in Fig. 5. A kicker magnet was

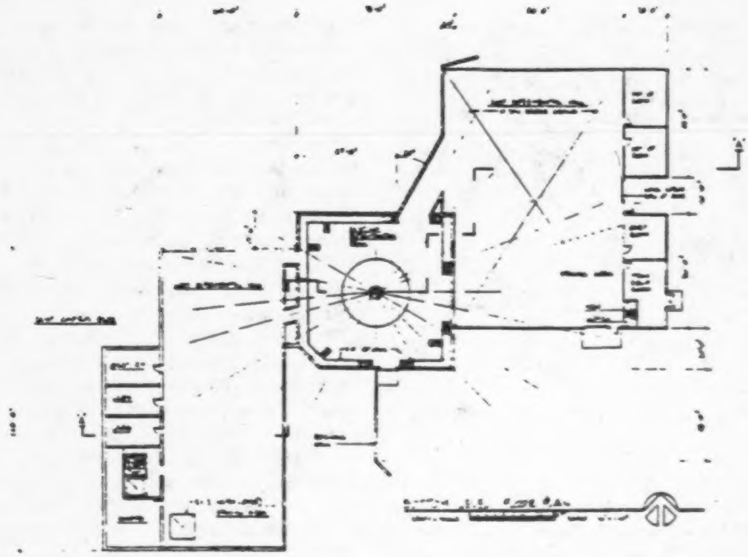

Fig. 3.
Lower level floor plan for experimental halls.

inserted into Line D to divert LAMPF 800-MeV macropulses into Line E with current initially at ~20 μA, upgradable to perhaps 200 μA. The beam line consists of four quadrupole doublets, two bending dipoles, a graphite target, and a tungsten beam stop. The target station is followed by a 12-m-long, 4-m-diam pion-decay tunnel and an iron-concrete shield approximately 9 m thick. The detector sits on a concrete pad beyond the iron shield in a concrete blockhouse used for cosmic-ray attenuation. Biological shielding is provided by concrete and earth overburden.

The target and beam-stop areas are water cooled and designed for remote handling. Iron shielding around the target allows manual maintenance to within a few feet of the target. The target is viewed by a beam pipe at 9° that allows one to monitor the pion flux continuously during the run.

Engineering for the construction and beam-line components was performed by Los Alamos Groups ENG-2 and P-12, construction was carried out by the Zia Corporation, and alignment was done by the Antares alignment crew (Group P-5). Beam-line magnets and power supplies were provided by LAMPF. Various beam components were fabricated or provided by university groups: vacuum pieces and electronics trailer (New Mexico State University); harp boxes (Temple University); target and computer (University of California, Riverside); and pion monitor (UCLA). Shielding material was provided by LAMPF and P Division.

A number of features incorporated into Line E will be used in future beam lines. The kicker magnet, its power supply, and the vacuum fan-out pipe will be duplicated for the PSR. The skew in Line E is a first at LAMPF and required a novel method of alignment, sighting along the bore tubes of the magnets. The harps for beam monitoring in Line E also are of a new design that will be duplicated for use in the PSR and other LAMPF beams.

The expected flux of muon neutrinos in the detector for a current of 20 μA is shown in Fig. 6. Provision has been made for a magnetic pion-focusing device that will be inserted just downstream of the target; it will enhance the neutrino flux by an order of magnitude. Flux calculations were performed using two Monte Carlo programs based on pion yields that were measured for carbon targets.

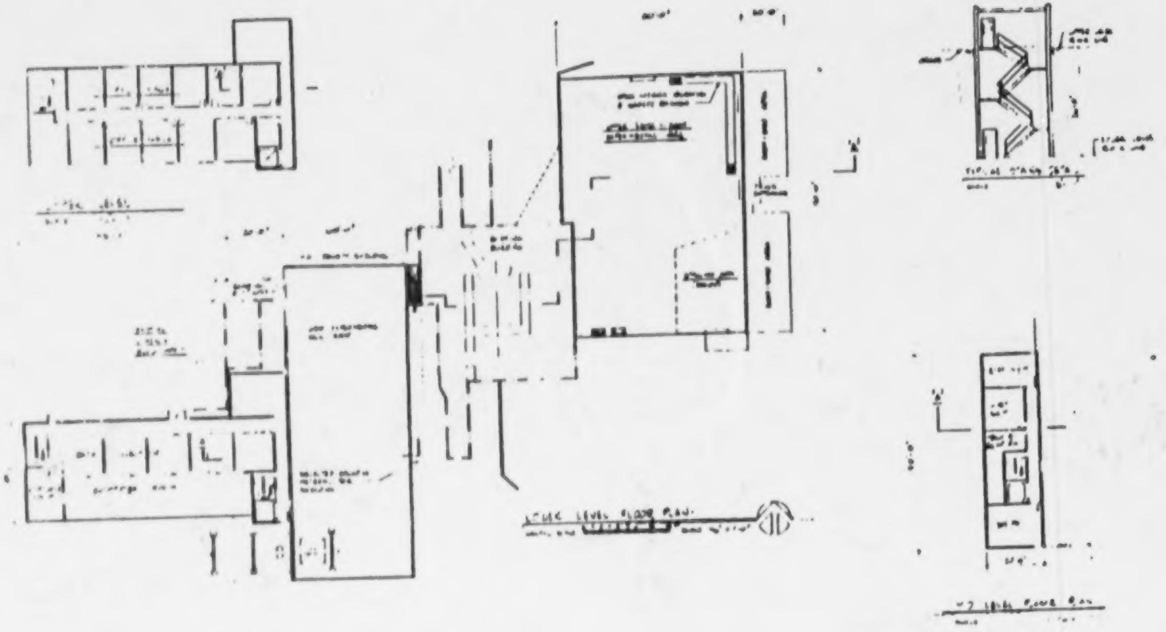

Fig. 4.
Upper level floor plan for experimental halls.

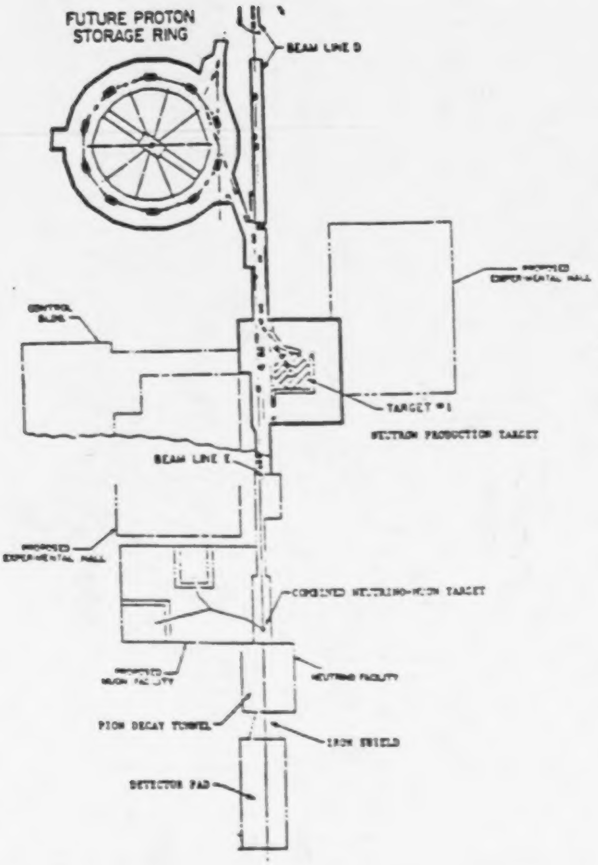
FUTURE PROTON
STORAGE RING
BEAM LINE D
PROPOSED
EXPERIMENTAL HALL
CONTROL
BLDG.
TARGET #1
NEUTRON PRODUCTION TARGET
BEAM LINE E
PROPOSED
EXPERIMENTAL HALL
COMBINED NEUTRINO-MUON TARGET
PROPOSED
MUON FACILITY
NEUTRINO FACILITY
PION DECAY TUNNEL
IRON SHIELD
DETECTOR PAD

Fig. 5.

Layout of the WNR/PSR complex showing location of neutrino beam line (Line E), neutrino-production target, pion decay channel, shielding, and neutrino detector.

At the end of 1983, the construction is approximately two-thirds complete. Beam-line magnet elements and a vacuum system are installed and tested, and alignment is complete, as are the wire connections. A test to transport a small proton current was successfully performed in January 1984.

Publication

1. P. Denes et al., Phys. Rev. C 27, 1339 (1983).

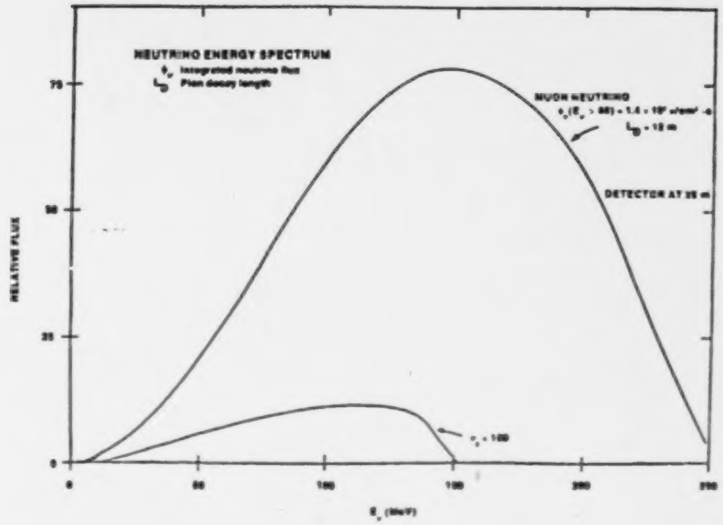

Fig. 6.
Calculated neutrino energy spectrum. Calculated flux is for a bare target with 20-μA beam of 800-MeV protons.

Research Programs

WNR/PSR Neutron Scattering Research

R. N. Silver, R. Alkire, G. Christoph, J. Eckert, J. Goldstone, A. Larson, R. Robinson, P. Seeger, P. Vergamini, and A. Williams

In 1983 the neutron-scattering group (P-8) announced a National User Program at the WNR/PSR facility. This announcement formally opened the facility to the national and international scientific communities in solid-state physics, chemistry, materials science, and biology. Proposals for the use of neutron-scattering instrumentation are reviewed by a nationally appointed Program Advisory Committee, which also reviews proposals for the Intense Pulsed Neutron Source (IPNS) at the Argonne National Laboratory. Proposals are reviewed on the basis of scientific excellence and optimal use of WNR/PSR characteristics.

The first two instruments in the formal User program are the Be-BeO Filter Difference Spectrometer (FDS) and the Single-Crystal Diffractometer (SCD). The FDS, shown in Fig. 7, is used for chemical spectroscopy, localized modes, and phonon density-of-state measurements. The FDS instrument is the responsibility of J. Eckert. The SCD, shown in Fig. 8, uses the Laue-TOF technique and is the responsibility of P. Vergamini. In 1983, 24 proposals for experiments were received and 15 were approved by the Program Advisory Committee.

In 1984 the Neutron Powder Diffractometer (NPD) will join the User program. The NPD is used for neutron powder diffraction by the Rietveld profile-refinement technique. The scientist responsible for the NPD is G. Christoph.

In 1983 major progress was made in the construction of neutron-scattering instrumentation. The present arrangement of instrumentation at the WNR is shown in Fig. 9.

(1) The prototype FDS and SCD instruments were completely rebuilt into well-engineered instruments suitable for the National User Program. These modifications greatly improved instrument performance and reliability.

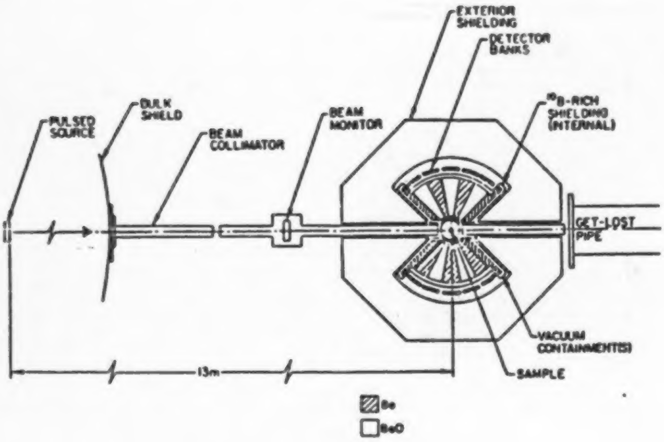
EXTERIOR SHIELDING
DETECTOR BANKS
^{10}B-RICH SHIELDING (INTERNAL)
PULSED SOURCE
BULK SHIELD
BEAM COLLIMATOR
BEAM MONITOR
GET-LOST PIPE
VACUUM CONTAINMENT(S)
SAMPLE
13m
Be
BeO

Fig. 7.
Filter Difference Spectrometer.

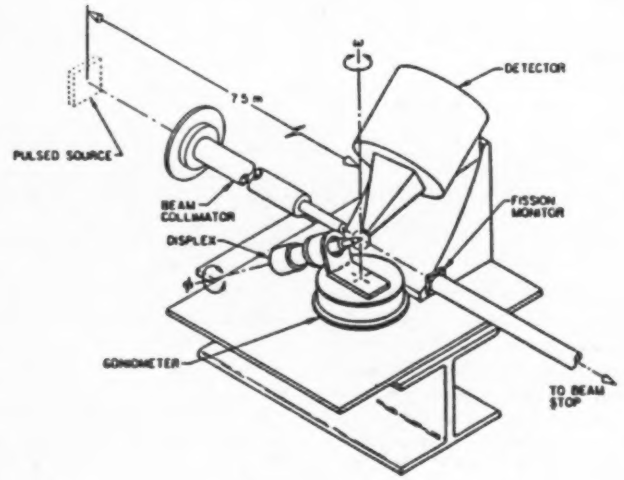
ω
DETECTOR
7.5 m
PULSED SOURCE
BEAM COLLIMATOR
FISSION MONITOR
DISPLEX
φ
GONIOMETER
TO BEAM STOP

Fig. 8.
Single-Crystal Diffractometer.

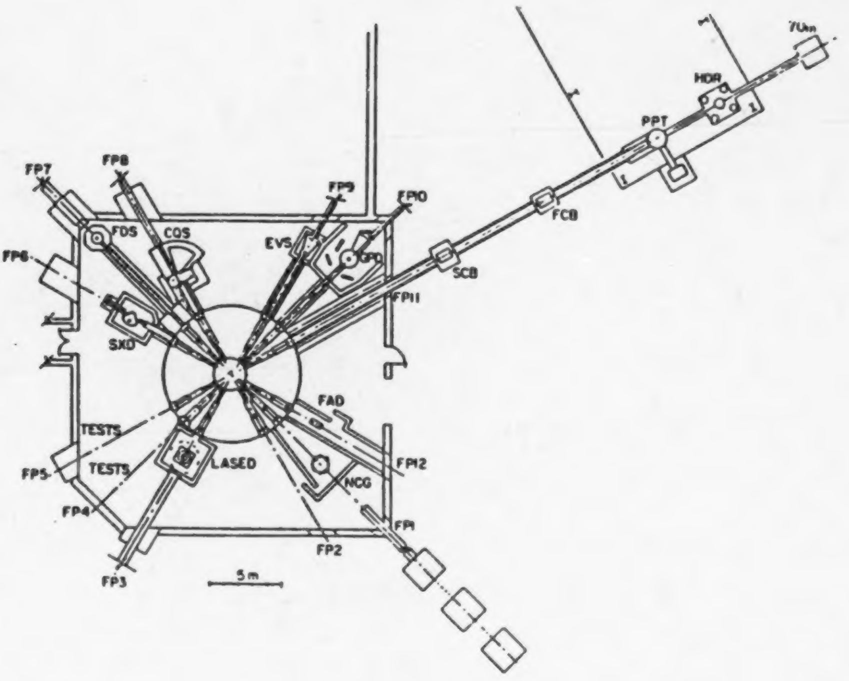

Fig. 9.
WNR layout of instrumentation.

(2) A prototype Constant-Q Spectrometer (CQS) began operation. The CQS, shown in Fig. 10, will be used to study elementary excitations, such as phonons and magnons in single-crystal samples.

(3) The nuclear-resonance-filter difference technique for electron-volt spectroscopy was extended to low-Q measurements appropriate for the study of magnetic and electronic excitations. In a collaboration with the Rutherford Appleton Laboratory, a prototype low-Q electron-volt spectrometer (EVS) was constructed and brought into initial operation at the WNR.

(4) An instrument optimized for low-angle diffractive scattering with epithermal neutrons at high intensities and low resolution is required for diffraction of liquids and amorphous materials. Such an instrument requires special attention to keep backgrounds low. A protoype diffractometer for liquid, amorphous, and special-environment materials (LASED) built with these goals in mind began operation at the WNR.

(5) A new sample environment container was constructed for the NPD, and additional detectors were installed.

Some highlights of neutron-scattering research in 1983 included the following.

- *First Molecular Hydrogen Complex*

  P. Vergamini and A. Larson (P-8) and H. Wasserman and R. Ryan (INC-4)

  The structure of the first complex that reversibly binds molecular hydrogen was determined by single-crystal neutron diffraction at the WNR facility. This is an intermediate species in the catalysis of hydrogen, a long-sought missing link. The structure is shown in Fig. 11.

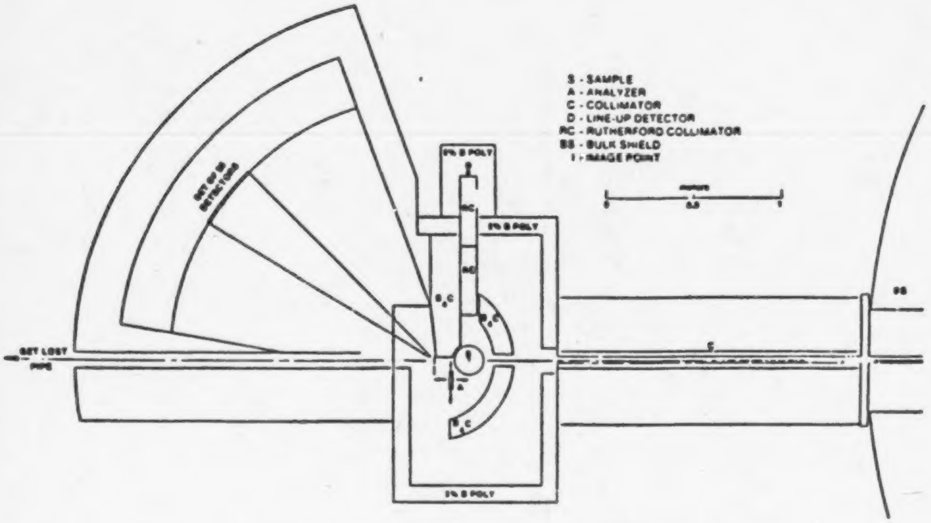
S - SAMPLE
A - ANALYZER
C - COLLIMATOR
D - LINE-UP DETECTOR
RC - RUTHERFORD COLLIMATOR
BS - BULK SHIELD
I - IMAGE POINT
0
0.5
1
5% B POLY
5% B POLY
5% B POLY
SET OF 32 DETECTORS
D
RC
RC
B₄C
B₄C
B₄C
S
I
A
BS
GET LOST PIPE

Fig. 10.
Schematic of the Los Alamos Constant-Q Spectrometer.

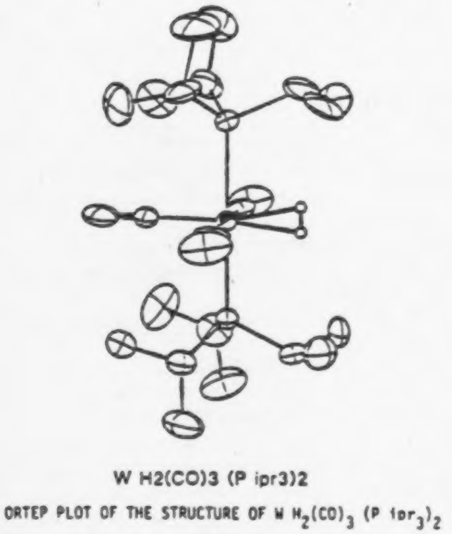
W H2(CO)3 (P ipr3)2
ORTEP PLOT OF THE STRUCTURE OF W H₂(CO)₃ (P ipr₃)₂

Fig. 11.
Molecular hydrogen complex.

- ***High-Pressure Structure of ReO$_3$***
  R. Alkire, A. Larson, J. Schirber, and B. Morosin (Sandia National Labs.)

  ReO$_3$ is an unusual material because it undergoes a "compressibility collapse" at high pressures with a factor-of-10 decrease in compressibility above 10 kbar. The long-sought structure of the high-pressure phase has finally yielded to a time-of-flight neutron-scattering experiment in which one can take advantage of the strong penetrating power of the neutron and its ability to Bragg scatter at fixed angles with a white neutron beam in a high-pressure (15-kbar) cell using the SCD.

- ***Hydrogen Sites in PbO$_2$ Battery-Plate Material***
  J. Eckert, J. Goldstone, J. Jorgensen, and R. Varma (Argonne National Lab.)

  The problem of hydrogen bonding in electrochemical cells is of immense practical interest. The strong penetrating power of the neutron, its sensitivity to hydrogen, and the high epithermal flux of the WNR facility make it a very suitable probe for addressing practical problems of this sort. Figure 12 shows inelastic neutron spectra taken with the Filter Difference Spectrometer of PbO$_2$ before and after

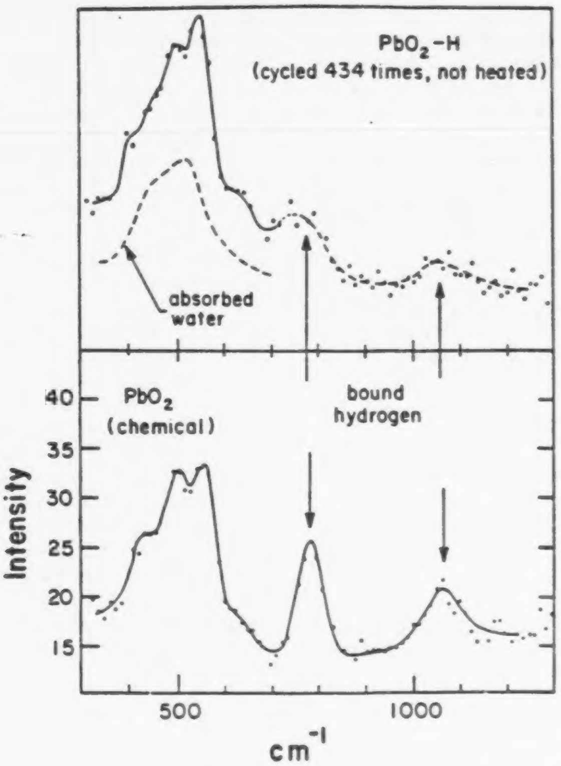

Fig. 12.
Inelastic neutron spectra of lead dioxide PbO$_2$ battery-plate material.

cycling. The spectra clearly show that the hydrogen introduced in the cells appears as vibrational modes of water H_2O and not as increased bound-hydrogen modes.

- ***Octahedral-Site Occupancy in Rare-Earth Hydrides** J. Goldstone, J. Eckert, G. Venturini, and P. Richards (Sandia National Labs.)*

  In LaH_x, CeH_x, and other rare-earth hydrides, the hydrogen atoms primarily occupy tetrahedral sites until $x > 2$ is reached, at which point octahedral sites begin to be filled. The relative occupancy of these sites can be determined by the differing vibrational modes in inelastic neutron scattering and by powder diffraction. In YH_x, octahedral sites were found to be occupied before $x = 2$ composition was reached, and the occupation of these sites increased with decreasing temperature, in contradiction to expectations of increasing order at low temperatures. Experiments at the WNR using the FDS and NPD instruments showed that the "octahedral" sites were not quite octahedral as the temperature decreased, leading to an increased degeneracy that could explain the observed temperature dependence.

Other important activities in the neutron-scattering group in 1983 included the following.

- *Development of a Proposal for the Expansion of the Experimental Halls at the WNR Facility.* In accordance with the recommendations of the DOE review committees (Brinkman I and II, and Rowe), a proposal has been developed and submitted to the

DOE for expansion of the experimental halls, computer support, and instrumentation in order for the WNR/PSR to serve as a national User facility. This proposal was submitted for FY 1985 funding.

- *Workshops and Conferences.* A workshop was held in September 1983 on "Frontiers in Condensed Matter Physics with the WNR/PSR Pulsed Neutron Source," chaired by R. Birgeneau of MIT. A mini-workshop was held in November on "Biological Applications of the WNR/PSR Facility." Planning was carried out for a conference to be held in February 1984 on "High-Energy Excitations in Condensed Matter," and commitments were made to sponsor an "International Conference on Neutron Scattering" in August 1985 in Santa Fe.

WNR/PSR Nuclear Science

Search for Resonance Structure in Few-Nucleon Systems

P. W. Lisowski and G. F. Auchampaugh (P-3); M. Moore and G. Morgan (P-15); and R. Shamu (Western Michigan Univ.)

During the past few years, both experimental claims and theoretical predictions for the existence of dibaryon resonances have been made. The conventional meson approach interprets observed structure in the nucleon-nucleon system as resulting from inelastic channels in various partial waves. A more exciting possibility is that the resonances may result from six-quark bound states. In this model the nucleons are pictured as two bags of quarks, with the resulting overlap producing a rich density of dibaryon states. Before experiments performed at Los Alamos in 1982 and 1983, there was no undisputed picture of the energy or width of the proposed resonances. In fact, searches at LAMPF and elsewhere had insufficient energy resolution to observe the narrow structure predicted by some models.

A search for resonance structure in the nucleon-nucleon system was completed by performing a high-resolution, high-precision *np* total cross-section measurement over the entire range of interest. These data showed no evidence for narrow structure. A broad anomaly previously seen in the *np* system, attributed to an $I = 1$, ${}^3F_3$ dibaryon resonance, was confirmed. An $I = 0$, ${}^1F_3$ state proposed by other authors was not observed. From 200 to 700 MeV, our data (Fig. 13) indicate that existing cross sections may be as much as 6% too low.

A second set of measurements searching for resonance effects in the nine-quark system *nD* was partially completed in 1983. These data will provide accurate cross sections to test both the theory of binding effects in the

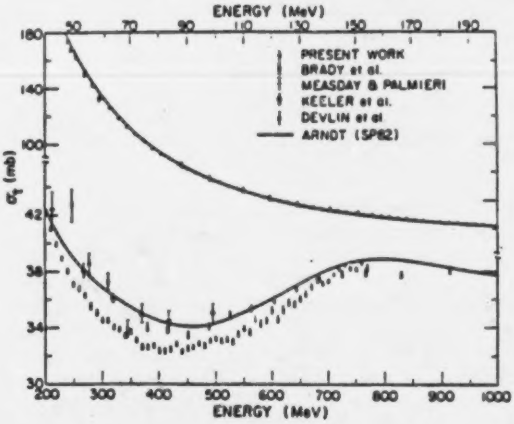

Fig. 13.

Comparison of present results with selected high-accuracy *np* total cross-section data and with phase-shift predictions. The upper (lower) data correspond to the upper (lower) energy scale. Note that the cross-section scale for the upper data is a factor of 10 smaller than that for the lower data.

deuteron and charge-symmetry effects in the three-nucleon system.

REFERENCE

1. P. W. Lisowski, R. E. Shamu, G. F. Auchampaugh, N. S. P. King, M. S. Moore, and T. S. Singleton, "Search for Resonance Structure in the *np* Total Cross Section Below 800 MeV," Phys. Rev. Lett. 49, 255 (1982).

High-Resolution Nucleon-Induced Charge-Exchange Reaction Studies at 800 MeV

P. Lisowski (P-3); G. Morgan and N. King (P-15); and P. Craig, D. Lind, R. Jeffesen, J. Shepard, J. Ullman, and C. Zafiratos (Univ. of Colorado)

Nucleon-induced charge-exchange reactions at bombarding energies of several hundred MeV have indicated that there are interesting but poorly understood processes involved. For example, in (p,n) reactions the strength of Gamow-Teller (GT) transitions may be computed from a simple sum rule. Recent data near 200 MeV indicate that approximately 30% of the expected GT strength is missing.

One exciting possibility is that the GT strength is "quenched" because of appreciable delta-isobar, nucleon-hole (Δ-hole) components in the low-lying GT levels. Such a theory, if correct, would imply that nucleon excitations such as the Δ, which have been considered to be too high in energy to be of importance in the low-energy domain, must be considered. Alternative conventional nuclear-structure effects also have been proposed to account for the GT quenching effect. Our studies of (p,n) reactions at the WNR will permit a search for the transfer of GT strength directly.

To study this and other aspects of nucleon-induced charge-exchange, we are using a 213-m-long 0° reaction angle flight path at the WNR, the only facility in the world capable of neutron energy resolution sufficient to permit the observation of nuclear-structure effects at 800 MeV. Preliminary results thus far obtained for (p,n) indicate that we can obtain information addressing four areas of interest: (1) the excitation of discrete levels leading to unique information on the isovector and isovector spin-flip parts of the effective *NN* interaction; (2) the nature of the Pauli-blocked quasi-elastic knock-on peak; (3) the nature of the broad resonances associated with the Δ and the possible implications for Δ-hole configurations in nuclear spectra; and (4) the excitation of charge-exchange analogs specifically using (n,p) reactions.

As an example of the above, we have compared our spectra for $^{13}C(p,n)$, shown in Fig. 14, with those available at lower energies and have conclusively identified GT and Fermi transitions, thus greatly extending the energy range over which these transitions have been studied.

To obtain angular distributions, we plan to install a beam swinger to change the angle of incidence of the proton beam and thereby obtain angular distributions using the existing equipment.

Neutron-Induced γ-Ray Processes

S. A. Wender and G. F. Auchampaugh (P-3); L. R. Nilsson (Tandem Accelerator Lab., Uppsala, Sweden); and N. R. Roberson (Triangle Universities Nuclear Lab., Duke Univ.)

Experiments that study γ rays in the energy range from 4 to 30 MeV produced by fast-neutron-induced reactions have been hampered by low data-acquisition rates, restricted neutron energy ranges, and high backgrounds. Typical systems for studying fast-neutron-capture reactions, for example, have been located at Van de Graaff accelerators and have used large-volume NaI detectors with massive active and passive shielding. These detector systems have been limited to one or two detectors because of their large size and high costs. The neutron sources have been limited in their energy range and resolution because they usually relied on secondary production targets [for example, the $D(d,n)$ reaction with gas cells].

During FY 1983 we developed a unique system to study high-energy γ rays produced by neutron-induced reactions. This system consists of five bismuth germanate (BGO) scintillators used in conjunction with a pulsed spallation neutron source at the WNR. The simultaneous acquisition of γ-ray excitation functions and angular distributions for incident neutrons in the energy range from 1 to 200 MeV is possible with this system (a paper describing this method has been accepted for publication in Nuclear Instruments and Methods). Figure 15 shows a diagram of the apparatus.

The physics program based on this system is being formulated as the particular parameters and capabilities of the system are determined. The program presently

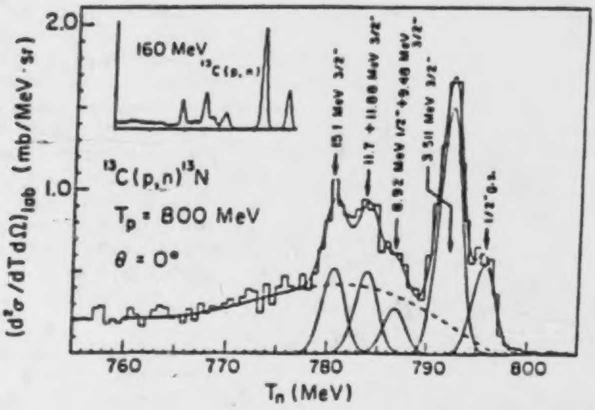

Fig. 14.

An 800-MeV $^{13}C(p,n)$ TOF spectrum at $\theta = 0°$. Overall resolution is approximately 2.5 MeV (FWHM). Arrows indicate expected locations of peaks observed in the 160-MeV spectrum shown in the inset. The smooth curves indicate best fits to the background and peaks.

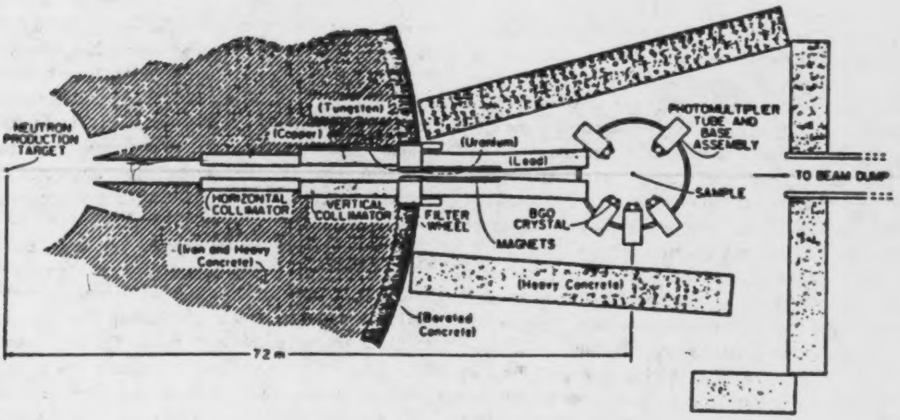
NEUTRON PRODUCTION TARGET
(Tungsten)
(Copper)
(Uranium)
(Lead)
PHOTOMULTIPLIER TUBE AND BASE ASSEMBLY
TO BEAM DUMP
SAMPLE
HORIZONTAL COLLIMATOR
VERTICAL COLLIMATOR
FILTER WHEEL
BGO CRYSTAL
MAGNETS
(Iron and Heavy Concrete)
(Heavy Concrete)
(Borated Concrete)
72 m

Fig. 15.

Experimental setup showing neutron collimators, shielding, and detector assembly.

consists of studying two broad areas: (1) inelastic neutron excitation of γ rays from bound states using the (n,n') reaction, and (2) fast-neutron-capture reactions into the giant-resonance region of nuclei.

In addition to these two programs we are also investigating the properties of the BGO detectors to optimize their characteristics.

Inelastic γ-Ray Production. As an initial test of the system, we measured the $^{12}C(nn'\gamma = 4.44\text{-MeV})$ reaction cross section for incident neutron energies from threshold (4.9 MeV) to 100 MeV. This reaction previously has been studied up to 20 MeV. Figure 16 shows the results of our measurements. These data represent approximately 13 h of beam time.

In this run we used only four BGO detectors at θ_{lab} = 55, 90, 125, and 140°. The data from these detectors were fitted to an expansion in Legendre polynomials,

$$d\sigma(\theta)/d\Omega = A_0\{1 + \Sigma a_k P_k[\cos(\theta)]\} \ .$$

The a_2 coefficient to the order of $k = 2$ as a function of neutron energy agrees well with previous results, and is shown in Fig. 17. However, the data show the need for terms to the order of $k = 4$, consistent with the results of the $^{12}C(p,p'\gamma = 4.44\text{-MeV})$ reaction. Because only four detectors were used and two of them were at symmetric angles, the errors in the Legendre coefficients are large when the expansion includes $k = 4$ terms; a remeasurement is planned.

Fast-Neutron Capture. For our first fast-neutron-capture experiment we studied the $^{40}Ca(n,\gamma_0)$ reaction. Because the cross section for this reaction in the giant-resonance region is only on the order of 10 μb, we used a relatively large sample of natural calcium (500 g, 7.6 cm long by 7.6 cm diameter). Data were acquired for approximately 50 h. Preliminary analysis of the ground-state γ-ray yield as a function of neutron energy, corrected for incident neutron flux and neutron energy bin size, is

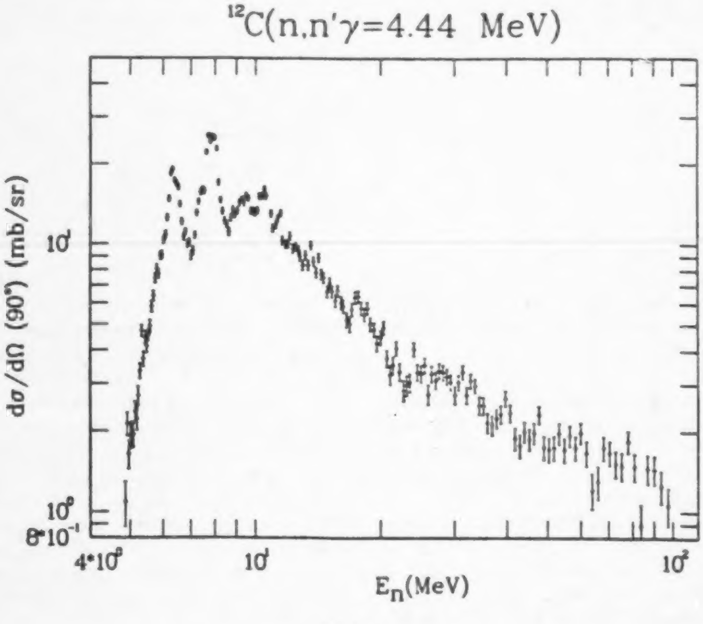

Fig. 16.
The 90° differential cross section for the $^{12}C(n,n'\gamma) = 4.44\text{-MeV}$ reaction as a function of neutron energy.

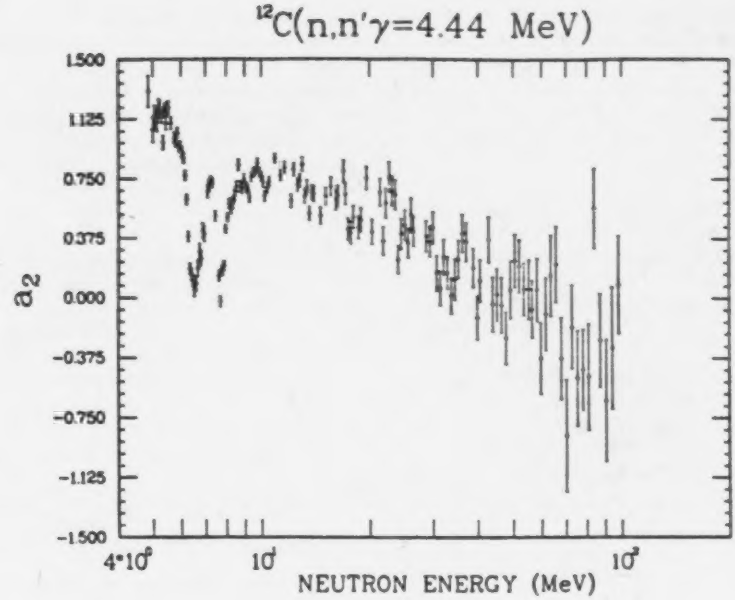

Fig. 17.
The A_2 Legendre polynomial coefficient for the 4.44-MeV γ ray from the $^{12}C(n,n'\gamma)$ reaction. The plot corresponds to fitting the data to A_0 and A_2 only.

shown in Fig. 18. The absolute cross section was obtained by normalizing to previous results. The maximum in the yield curve at $E_n = 11$ MeV corresponds to the peak of the giant dipole resonance in ^{41}Ca. The shape of this excitation function is in good agreement with previous results.

BGO Detector Development. The use of BGO scintillators to detect high-energy γ rays is a relatively recent development. We therefore have spent some time studying their characteristics and have considered methods to improve their performance.

In a paper submitted to Nuclear Instruments and Methods, we report the measurement of absolute efficiency of a 7.6- by 7.6-cm BGO detector at 15 MeV. We used the $^{12}C(p,\gamma_0)$ reaction at $E_p = 14.2$ MeV and determined the efficiency to be (51 ± 4)%. We expect to obtain response functions and efficiencies over the energy range 1-30 MeV.

Planned Work. We plan to continue our study of the $^{12}C(n,n'\gamma)$ reaction to improve the quality of the preliminary data, and to study ^{11}B, which shows several isolated resonances in the γ-ray yield for the 2.0- and 4.4-MeV states. In addition, we plan to measure the γ-ray production cross section of ^{14}N and ^{15}N.

The fast-neutron-capture program will continue the study of the giant-resonance region of nuclei — in particular, the search for the isovector $E2$ resonance in ^{208}Pb. In addition, we plan to search for giant resonances built on excited states in ^{14}C using the $^{13}C(n,\gamma)$ reactions. Such resonances previously have been seen in proton-capture studies. Visitors interested in participating in this research are welcome.

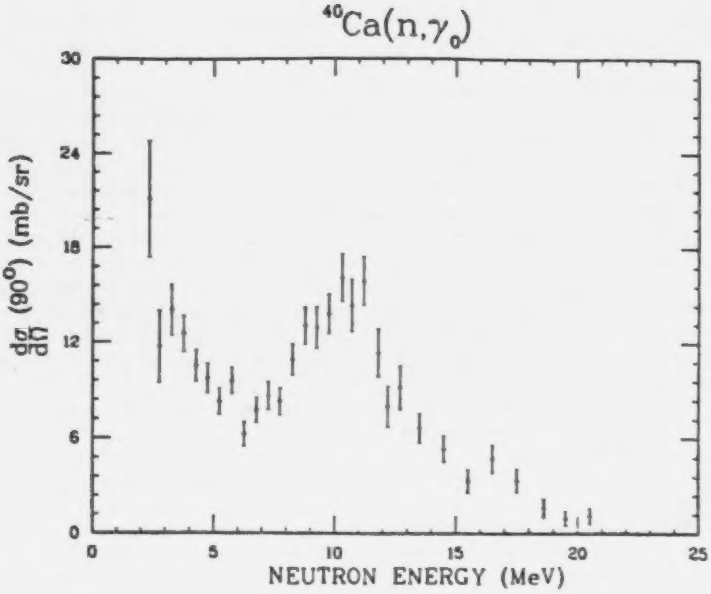

Fig. 18.
The 90° differential cross section for the ^{40}Ca(n,γ_0) reaction as a function of incident neutron energy.

Fission Fragment Angular and Kinetic Distributions for Actinide Nuclei

G. F. Auchampaugh (P-3); M. S. Moore (P-15); C. E. Olsen (MST-13); C. Goulding (Q-2); N. W. Hill (Oak Ridge National Lab.); and R. White (Lawrence Livermore National Lab.)

Angular, kinetic-energy, and mass distributions as functions of excitation energy play an important role in revealing the physics of the fission process. Answers to questions such as the importance of shell effects and angular momentum on the potential energy surface, the nature of vibration and complex structures associated with this surface, and the time scale and energy dissipation mechanism in fission are all addressed by such measurements. The paucity of high-quality data in this area opens a rich field of research in neutron physics.

During the past year we developed a double-volume Frisch-grid ionization chamber that permits simultaneous measurements of the angular, kinetic-energy, and mass distributions of each fragment as a function of neutron energy for low α-active targets. A detector with cathode foils of ^{233,238}U and ^{232}Th was used to obtain data from 0.8 to 20 MeV at the WNR facility. The ^{235}U data have been examined in detail and show systematic effects that are attributed to nonuniformity in the conductivity of the foils and base-line shifts because of pulse pileup from charged particles in the neutron beam. Further development and measurements are planned.

On the Nature of the Coupling in Subthreshold Fission of ^{238}Np

G. F. Auchampaugh and J. D. Moses (P-3); M. S. Moore (P-15); R. O. Nelson (P-9); R. C. Extermann (P-3 Visiting Staff Member); C. E. Olsen (MST-13); and N. W. Hill and J. A. Harvey (Oak Ridge National Lab.)

Although intermediate structure in subthreshold fission was first observed in the neutron-induced fission of ^{237}Np (Refs. 1 and 2), and the structure at 40 eV has been extensively studied,[3,4] the nature of the coupling between the first and second wells of the ^{238}Np fission barrier remains unknown.

Inspection of high-resolution fission data[4] reveals that several levels are strongly enhanced in the fission channel, so that the mixing between the class II level underlying the intermediate structure and the class I background is neither extremely weak nor very strong. The mixing can, however, be attributed to two very different physical causes, as discussed by Bjørnholm and Lynn.[5] In the simplest case, the two classes of states may be weakly mixed because of a high intermediate barrier. Bjørnholm and Lynn refer to this kind of mixing as moderately weak mixing to a narrow class II state. Alternatively, the class II state may have a very large fission width that leads to weak mixing because of rapid decay of the class II state. This is known as very weak mixing to a broad class II state. The data for ^{237}Np have not clearly distinguished between these alternatives.

Our work was an attempt to resolve this question by measuring the fission and total cross sections with very good energy resolution (1) to expose any underlying broad resonance near 40 eV, if possible; and (2) to obtain good enough resonance parameters to permit detailed analysis of the fine structure of the class II fission resonances at 40 and 120 eV.

The total cross section was measured at the Oak Ridge Electron Linear Accelerator using a 78-m flight path and metallic samples cooled to liquid-nitrogen temperature (~77 K) to reduce Doppler broadening. The fission cross section was measured at the WNR using a 30-m flight path and a unique cryogenic ionization chamber that maintained the samples at a temperature of 84 K. Both experiments were designed to achieve the highest statistical accuracy and the smallest possible neutron resolution at the 40- and 120-eV class II states.

We attempted to determine the relative sizes of the coupling and fission widths of the subthreshold resonances in ^{238}Np by measuring and analyzing the fission and total cross sections with great care and by analyzing the resulting resonance parameters by a variety of techniques. We believe we succeeded to the extent that we carried these techniques as far as they can reasonably be taken with current technology. We did not succeed in providing a clear answer to the nature of the coupling in ^{238}Np.

The multilevel analysis neither requires nor precludes the presence of a broad resonance underlying the 40-eV structure. The statistical analysis of the resonance-spacing distribution gives some indication that an anomalous intruder level is present at 40 eV, but the data also permit the alternate hypothesis. We believe that this problem will not be resolved by precise measurements of the type described here, but by a more sensitive measurement of a different type that can be carried out at the WNR.

6.2 Los Alamos Equation of State Library Center

1. For the period FY 1981 (or from start of operation) - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).

Answer: MATERIALS SCIENCES SUBPROGRAM
(Budget Authority in Thousands)

FY	Operations	In-House Research
85 (estimated)	0	0
84	$125	$125
83	$120	$120
82	$125	$125
81	$140	$140

2. How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?

Answer: No direct funding was provided by other federal agencies, or is expected.

3. What facility changes and additions have occurred or are anticipated for the period FY 1981 (or from start of operation if later) - FY 1985?

Answer: The purpose of the Library is to provide high quality equation of state data to users in the form of a data base. Consequently, this is a theoretical effort with no need for special facilities except an existing computer center; thus there are no facility changes or additions. DOE is terminating support for this center in FY 1985 due to insufficient user demand to make the facility cost effective.

4. For the period FY 1981 (or from start of operation) - FY 1985, please provide actual and estimated staffing levels.

Answer: The staffing level supported by Materials Science is below. Support for this center is being terminated in FY 1985 as a result of insufficient user demand to make the center cost effective.

FY	Staffing Level (FTE)
1985	0
1984	2
1983	2.2
1982	2.2
1981	3.0

5. **What is the actual and estimated facility utilization for the period FY 1981 or from start of operation) - FY 1985? What would be defined as "full" utilization of the facility?**

   Answer: This is difficult to answer since tangible property is not involved but our best estimate is that full utilization is being achieved for all potential use. By "full utilization" it is meant that all available time on the facility is occupied. DOE is terminating support for this center in FY 1985 as a result of insufficient user demand to make the Center cost effective.

6. **What is this facility's user policy?**

   Answer: The present policy is to furnish the data base to any user upon request. We only ask that they supply the blank computer types. Since we are losing our support, we are, for FY 1985, instituting a small fee to recover some of our expenses.

7. **How many university personnel (i.e., faculty and students) have utilized the facility over the past five years (or from start of operation)?**

   Answer: We have eighteen university users and eighteen in other national laboratories for a total of 36 users.

8. **How many industrial researchers have utilized the facility over the past five years (or from start of operation)?**

   Answer: We have nineteen industrial users.

9. **How many researchers from foreign institutions have utilized the facility over the past five years (or from start of operation)?**

   Answer: We have twenty users at foreign institutions.

10. **What are the future development possibilities for this facility, what plans are being made to exploit these possibilities, and what are the budgetary implications?**

    Answer: Support for this Center is being terminated in FY 1985 as a result of insufficient user demand to make the Center cost effective.

11. **Please provide a copy of the facility's latest annual report.**

    Answer: See attached.

DOE F 5120.2
(6-80)

U.S. DEPARTMENT OF ENERGY
FIELD TASK PROPOSAL/AGREEMENT

1. WORK PACKAGE NUMBER	2. TASK NO.	3. REV. NO. 0	4. PROJECT NO.	5. DATE PREPARED 04/01/83	6. CONTRACTOR NUMBER E421

7. TASK TITLE: Los Alamos Equation of State Library

8. WORK PACKAGE TITLE:

9. BUDGET AND REPORTING CODE: KC-02-02-03-0

10. TASK TERM Begin: End: Open

11. CONTRACTOR NAME: Los Alamos National Laboratory

12. CODE (See instructions)

13. CONTRACTOR TASK MANAGER (Name: Last, First, MI) (FTS No.)

BELL, George I.
Theoretical Division Leader
FTS: 843-4401

14. PRINCIPAL INVESTIGATORS (Name: Last, First, MI)

ABDALLAH, J.; ALBERS, R. C.; BENNETT, B. I
DOWELL, F.; HOLIAN, B. L.; JOHNSON, J. D.;
LYON, S. P.; STRAUB, G. K.; TRAINOR, K.;
HUEBNER, Walter F.

15. WORK LOCATION (See instructions). Name of facility, City, State, Zip Code

Los Alamos National Laboratory
P. O. Box 1663
Los Alamos, NM 87545

16. Is this task included in the Institutional Plan? ☒ YES ☐ NO

17. Does this task include any management services efforts? ☐ YES ☒ NO

18. TASK DESCRIPTION (Approach, relation to work package, in 200 words or less)

Maintain a computer-based library of equations of state (EOS) and other related material properties for application to energy and general science programs. Survey current user requirements for the EOS and calculate or acquire and evaluate the needed data. Store EOS data in tabular form suitable for use in realistic hydrodynamic code calculations and other applications. Distribute data to users on magnetic tape in a universal computer format. Apply theories of solids, liquids, gases, plasmas, and mixtures to generation of EOS data. Develop new theoretical methods when existing theories and experiments are insufficient to satisfy user requirements.

19. CONTRACTOR TASK MANAGER

Bell
(Signature)

2/11/83
(Date)

20. DETAIL ATTACHMENTS (See instructions)

☐ a. Facility Requirements
☒ b. Publications
☒ c. Purpose
☒ d. Background
☒ e. Approach
☒ f. Technical progress
☒ g. Future accomplishments
☒ h. Relationships to other projects
☐ i. Environmental assessment
☐ j. Explanation of milestones
☐ k. ZBB Detail
☒ l. Other (Specify) See #20 l, Capital Equipment Funds

#20B PUBLICATIONS

The following are the publications from approximately the beginning of fiscal year 1982 to the present. Appendix A lists publications from 1979 through 1982. Many of these publications were not listed in previous proposals.

a. Journal Articles

R. C. Albers and J. E. Gubernatis, "Self-Consistent Phonon Approximations for the Solid Phase of a One-Component Plasma," Phys. Rev. B 23, 2782 (1981).

A. K. McMahan and R. C. Albers, "Insulating Nickel at a Pressure of 34 TPa," Phys. Rev. Lett. 49, 1198 (1982).

F. Dowell, "Ordered Phases of Rigid Cores Having Semiflexible Tails: I. General Model for Orientational and Positional Ordering with Hard Repulsions," Phys. Rev. B (submitted).

F. Dowell, "Ordered Phases of Rigid Cores Having Semiflexible Tails: II. Model for Smectic A and Reentrant Nematic Phases with Hard Repulsions," Phys. Rev. B (submitted).

F. Dowell, "Nematic-Isotropic Transition in Some Lattice Models for Rigid Cores Having Semiflexible Tails: Segmental Lennard-Jones Interactions," Phys. Rev. A (submitted).

D. C. Wallace, B. L. Holian, J. D. Johnson, and G. K. Straub, "High-Temperature Free-Energy Expansion for Metal Fluids," Phys. Rev. A 26, 2882 (1982).

B. L. Holian, D. C. Wallace, R. E. Swanson, and G. K. Straub, "Molecular Dynamics of the Melting of Sodium," Phys. Rev. B (to be published).

B. L. Holian and D. J. Evans, "Shear Viscosities away from the Melting Line: A Comparison of Equilibrium and Nonequilibrium Molecular Dynamics," J. Chem. Phys. (to be published).

D. A. Liberman, "INFERNO: A Better Model of Atoms in Dense Plasmas," J. Quant. Spectrosc. Radiat. Transfer 27, 335 (1982).

G. K. Straub, R. E. Swanson, B. L. Holian, and D. C. Wallace, "The Thermal Properties of Metallic Sodium Near Melt from Molecular Dynamics Calculations," in the Proceedings of the CECAM Workshop on "Ab Initio Calculations of Phonon Spectra," Antwerpen, Belgium, edited by Devreese, Van Doren, and Van Camp (Plenum, 1982).

R. E. Swanson, G. K. Straub, and B. L. Holian, "Molecular Dynamics of Sodium Using a Model Pseudopotential," in the Proceedings of the 1981 Topical Conference on Shock Waves in Condensed Matter, Menlo Park, W. J. Nellis, L. Seaman, and R. A. Graham, Eds., (American Institute of Physics, New York, 1982).

R. E. Swanson, G. K. Straub, B. L. Holian, and D. C. Wallace, "Thermodynamic Properties of Solid Sodium from Quasiharmonic Lattice Dynamics and Molecular Dynamics," Phys. Rev. B 25, 7807 (1982).

D. C. Wallace and G. K. Straub, "Ensemble Corrections for the Molecular Dynamics Ensemble," Phys. Rev. A 27 (March 1983).

K. Trainor, "Construction of a Wide-Range Tabular Equation of State for Copper," J. Appl. Phys. (to be published).

b. Abstracts for Meetings

R. C. Albers and J. E. Gubernatis, "Brillouin-Zone Integration Schemes: An Efficiency Study for the Phonon Frequency Moments of the Harmonic, Solid, One-Component Plasma," Bull. Am. Phys. Soc. 26, 281 (1981).

F. Dowell, "Dipolar Interactions for Liquid Crystal Cores with Semiflexible Tails," Bull. Am. Phys. Soc. 27, 355 (1982).

R. E. Swanson, G. K. Straub, and B. L. Holian, "Molecular Dynamics of Sodium Using a Model Pseudopotential," Bull. Am. Phys. Soc. 26, 662 (1981).

c. Reports

J. Abdallah, Jr., "User's Manual for CURVES," Los Alamos National Laboratory report LA-8844-M (October 1981).

R. C. Albers and J. E. Gubernatis, "Brillouin-Zone Integration Schemes: An Efficiency Study for the Phonon Frequency Moments of the Harmonic, Solid, One-Component Plasma," Los Alamos National Laboratory report LA-8674-MS (January 1981).

F. Dowell and J. D. Johnson, "A Simple EOS for Polytetrafluoroethylene (Teflon)," Los Alamos National Laboratory report LA-9439-MS (August 1982).

F. Dowell, "A Simple EOS for Branched (Low-Density) Polyethylene," Los Alamos National Laboratory report LA-9559-MS (October 1982).

F. Dowell, "A Simple EOS for "Linear" (High-Density) Polyethylene (Marlex)," Los Alamos National Laboratory report LA-9564-MS (November 1982).

J. D. Johnson and B. I. Bennett, "An EOS for Carbon Phenolic," Los Alamos National Laboratory report LA-9176-MS (March 1982).

J. D. Johnson and S. P. Lyon, "SES2D User's Manual," Los Alamos National Laboratory report LA-9164-M (April 1982).

E. H. Lieb and D. A. Liberman, "Numerical Calculation of the Thomas-Fermi-von Weizsäcker Function for an Infinite Atom without Electron Repulsion," Los Alamos National Laboratory report LA-9186-MS (April 1982).

Equation-of-State and Opacity Group, Theoretical Division, Los Alamos National Laboratory, "SESAME '83: Report on the Los Alamos Equation-of-State Library," Los Alamos National Laboratory brochure LALP-83-4 (February 1983).

d. Presentations

J. D. Johnson, "Sesame: A Tabular Equation-of-State Library," presentation to the Instituto Mexicano del Petroleo (February 1982).

Equation-of-State and Opacity Group, Theoretical Division, Los Alamos National Laboratory, "Sesame: A Library of Equations of State and Atomic Physics Data Bases," invited paper at the March 1983 American Physical Society meeting in Los Angeles.

#20C PURPOSE

An equation of state (EOS) describes the response of a material to mechanical and thermal stresses, using thermodynamic variables such as pressure and energy. EOS data are used in modeling physical processes which occur in many energy programs, such as the safety of nuclear reactors and tanks for liquefied natural gas and in basic and applied research such as astrophysics and planetary science. In the Sesame EOS library, EOS tables are stored on a computer file where they can be accessed by users for a wide variety of applications. The tables are sent from Los Alamos to other institutions on magnetic tapes, in a format which can be interpreted even if the other installation has a computing system different from that at Los Alamos. The Sesame EOS tables provide a standard, incorporating the best experimental and theoretical data.

#20D BACKGROUND

The Sesame EOS Library was developed at Los Alamos to provide data used in laboratory defense and energy programs. As early as 1972, our EOS for deuterium was sent outside the Laboratory for use in laser fusion research, and other data were sent to Livermore and to the Air Force Weapons Laboratory. Under current DOE funding, initiated in March, 1976, the Library was broadened to supply data to more groups outside Los Alamos. A new and more flexible data management scheme for generating, storing, and accessing EOS tables was designed. Methods for transmitting data to users on magnetic tapes, in a system independent format, were devised. Models for generating EOS tables have been developed, improved, and applied to new materials. Material properties such as opacities, conductivities, and mean ion charge have been added in 1980.

#20E APPROACH

Sesame EOS tables usually cover a much wider range of pressure and temperature than can be studied by experimental methods. To construct an EOS table, it is necessary to employ theoretical models of solids, liquids, vapors, and plasmas, for mixtures and chemical compounds as well as pure elements. A realistic EOS should include transitions between the different phases. All types of materials are studied, including gases, metals, ceramics, plastics, glasses, and even composites such as rocks and minerals.

The effort required to construct an EOS table involves compilation and analysis of data, application of theoretical methods, and evaluation of the results. The approach to be taken must be selected by compromising the conflicting requirements of speed and accuracy. For urgent requests, an EOS can be created in less than a week, although the product is crude. Occasionally, a full year may be devoted to generating an EOS table consistent with a very high standard.

When a new EOS has been created, it is stored in a tabular form which has been found to represent the data accurately over the entire range studied. In most cases, the user can begin to apply the new table to a problem without having to analyze, interpret, or adapt it to his particular needs. Information about the availability of new data is communicated to users by journal articles, reports, informal newsletters, and by personal contact.

EOS tables of high standard from sources other than Los Alamos even though of more restricted pressure-temperature ranges are also incorporated in the Library.

#20F PROGRESS IN FY82

The Equation of State Library has had a very good FY82. We have new users and a large number of new tables in the Library. We have a new brochure describing the Library and have started the documentation of the Library. We have been invited by Professor George H. Vineyard on behalf of the Division of Condensed Matter Physics of the American Physical Society to give a presentation at the March 1983 meeting of the American Physical Society in Los Angeles. The presentation will be given at the session on National Facilities of Importance to Condensed Matter Physics. It has been a very active year, as reflected in our publication list. The following give more details and list other progress.

a. Chemical Equilibrium
As promised last year, the electronic partition function and atomic energy level data have been included into the chemical equilibrium code. Also, for this code the JANAF tables of equilibrium data have been obtained from the Dow Chemical Corporation and placed on the Los Alamos computer system.

b. New Materials Added to the Library
We have added or made substantial alterations to 24 equation of state (EOS) tables. Notable among the EOS's produced by us are those for copper, aluminum, teflon, and three versions of polyethylene. We continued to obtain good EOS's from outside sources such as the National Bureau of Standards and Lawrence Livermore National Laboratory. Argon, helium, and ammonia are examples of such materials that were placed on the Library in the past year. Isobutane, n-butane and propane have been obtained from NBS but are not yet on the Library. Electrical and thermal conductivities for 14 materials and opacities for 26, all over extensive temperature and density ranges, have been calculated and placed on the Library. All these new tables are summarized in Appendix B.

In addition to the just described activity, we have added new EOS tables to the Library to contain the individual contributions of nuclear motion, electronic, and cold curve contributions to the EOS's. This is a two-temperature (2-T) capability of interest to, for example, laser fusion users. In all new EOS's, we have tabulated this new information plus the standard EOS information. For the older materials of the Library, a retrofitting method for the 2-T tables was developed; 31 materials have been so retrofitted.

c. New Users
The number of users (external of Los Alamos) who have requested the Library on tapes has grown to 50. Three old users requested and were furnished updates.

d. Presentations and Documentations of the Library
A new brochure, updating our old one, has been prepared and is in press. We presented the Library in a talk to the Instituto Mexicano del Petroleo. As mentioned in the introduction of this section, we will be giving a presentation on the Library before the American Physical Society. This will give us exposure before a large number of potential new users.

e. Nonspherically Symmetric Molecules (especially including orientational ordering)
Several improved theories for chain molecules in fluid phases and in partially ordered condensed phases were developed. These theories can be used to calculate the contributions from London dispersion interactions and dipolar interactions to the thermodynamic properties, phase behavior, and molecular ordering (orientational and/or positional) in systems of chain molecules, ranging from very short chains to liquid crystals and polymers. The molecules, which may have both rigid and partially flexible portions, have site-site intermolecular interactions. These theories are especially appropriate for treating molecules that have anisotropies in shape and intramolecular composition so large that (1) perturbation approaches applied to theories for more spherically symmetric molecules fail and (2) computer simulation approaches are somewhat prohibitive.

f. Nonspherically Symmetric Molecules (away from orientational ordering)
A new, highly accurate, technique for reducing the true nonisotropic potentials of molecules to effective spherical potentials was developed. This method is appropriate for the investigation of the thermodynamics of molecular substances away from orientational ordering transitions. It justifies the long-standing procedure of fitting molecular thermodynamic data with spherical potentials and is of great importance to the modeling of detonations. Papers are in preparation.

g. Electronic Structure
We have implemented a state-of-the-art, linear-muffin-tin-orbital (LMTO), electronic structure code. With such, we have discovered a new insulating phase of Ni, and calculated cold curves for Na and molybdenum.

h. Pseudopotentials and Molecular Dynamics
The study of the primary EOS properties, i.e., energy-temperature-volume relationships, secondary EOS properties, i.e., elastic moduli, expansion coefficients, Grüneisen parameters and transport properties of metals using pseudopotentials and molecular dynamics has made significant progress. This is reflected in the large number of papers, either published or in various stages of preparation.

#20G FUTURE ACCOMPLISHMENTS

We will be continuing the significant accomplishments of the past year. Some details follow.

a. We will continue to place new EOS's on the Library, both from outside sources and from our own work. In particular, we will tabulate the isobutane, n-butane, and propane, and we have plans for creating Li^6D, molybdenum, gold, and silver EOS's.

b. We will continue the ongoing documentation of the library and continue to seek new users. We will obtain additional exposure to new users through the 9th West Coast Statistical Mechanics Meeting, which we are hosting in June 1983.

c. The pursuit of primary and secondary EOS properties and of transport properties of metals through pseudopotentials and molecular dynamics will be continued. The fundamental techniques will be further developed and the studies will be extended to new materials and new properties.

d. It would appear that the mathematical technique for treating nonspherical molecular potentials with effective spherical potentials has implications for the mixing of fluids. We will pursue this thought.

e. The development and use of high-quality electronic structure calculations will continue. The cold curves for more materials, especially at high pressure, will be calculated. Work on developing the capability to treat electronic levels in dense plasmas and to study the electronic structure of clusters is anticipated.

f. The theories developed for nonspherically symmetric molecules will be improved and will be adapted to generate improved EOS tables for chain molecules and polymers in the Sesame Library, thereby attracting new users in various areas (as, for example, enhanced oil recovery researchers interested in hydrocarbon chains). We want to extend the theories to calculate EOS tables for planar molecules in partially ordered phases (structures important, for example, in coals).

The progress for FY82 was excellent. It is not clear that level will be repeated in FY83 because: (1) what can be called research progress in a report fluctuates markedly from year to year; and (2) in FY82 other projects were slighted in favor of working on the Library. To make more probable that progress on the Library continue at the current high level, it is essential that the requested funding be delivered.

#20H RELATIONSHIP TO OTHER PROJECTS

Our Group (T-4) has the responsibility to calculate equations of state and opacities for Los Alamos programs, which include weapons development, reactor safety, and inertial confinement fusion. The Group studies power loss in Tokamaks under another DOE-funded program. We have a NASA-funded project to study comet atmosphere chemical kinetics modeling. The Group is involved in studies of the EOS for detonation modeling and other EOS, opacity and conductivities at very high density. Isotope separation studies have been active for over a year.

#201 CAPITAL EQUIPMENT FUNDS

Our data analysis capabilities need to be further enhanced. Therefore, equipment funds of $22,000 are requested.

APPENDIX A

EQUATION OF STATE PUBLICATIONS
1979 - 1982

Journal Articles

R. C. Albers and J. W. Wilkins, "Spin Relaxation of ^{3}He to Paramagnetic Centers in Surfaces at Very Low Temperatures," J. Low Temp. Phys. 34, 105 (1979).

R. C. Albers and J. E. Gubernatis, "Self-Consistent Phonon Approximations for the One-Component Plasma," Bull. Am. Phys. Soc. 25, 349 (1980).

R. C. Albers and J. E. Gubernatis, "Brillouin-Zone Integration Schemes: An Efficiency Study for the Phonon Frequency Moments of the Harmonic, Solid, One-Component Plasma," Bull. Am. Phys. Soc. 26, 281 (1981).

R. C. Albers and J. E. Gubernatis, "Self-Consistent Phonon Approximations for the Solid Phase of a One-Component Plasma," Phys. Rev. B 23, 2782 (1981).

A. K. McMahan and R. C. Albers, "Insulating Nickel at a Pressure of 34 TPa," Phys. Rev. Lett. 49, 1198 (1982).

F. Dowell, "Ordered Phases of Rigid Cores Having Semiflexible Tails: I. General Model for Orientational and Positional Ordering with Hard Repulsions," Phys. Rev. B (submitted).

F. Dowell, "Ordered Phases of Rigid Cores Having Semiflexible Tails: II. Model for Smectic A and Reentrant Nematic Phases with Hard Repulsions," Phys. Rev. B (submitted).

B. L. Holian and G. K. Straub, "Molecular Dynamics of Shock Waves in Three-Dimensional Solids: Transition from Nonsteady to Steady Waves in Perfect Crystals and Implications for the Rankine-Hugoniot Conditions," Phys. Rev. Lett. 43, 1598 (1979).

B. L. Holian, "Cell-Model Prediction of the Melting of a Lennard-Jones Solid," Phys. Rev. B 22, 1394 (1980).

W. G. Hoover, A. J. C. Ladd, R. B. Hickman, and B. L. Holian, "Bulk Viscosity via Nonequilibrium and Equilibrium Molecular Dynamics," Phys. Rev. A 21, 1756 (1980).

B. L. Holian, W. G. Hoover, B. Moran, and G. K. Straub, "Shockwave Structure via Nonequilibrium Molecular Dynamics and Navier-Stokes Continuum Mechanics," Phys. Rev. A 22, 2498 (1980).

B. L. Holian, H. Flaschka, and D. W. McLaughlin, "Shock Waves in the Toda Lattice: Analysis," Phys. Rev. A 24, 2595 (1981).

D. C. Wallace, B. L. Holian, J. D. Johnson, and G. K. Straub, "High-Temperature Free-Energy Expansion for Metal Fluids," Phys. Rev. A 26, 2882 (1982).

B. L. Holian, D. C. Wallace, R. E. Swanson, and G. K. Straub, "Molecular Dynamics of the Melting of Sodium," Phys. Rev. B (1983).

B. L. Holian and D. J. Evans, "Shear Viscosities away from the Melting Line: A Comparison of Equilibrium and Nonequilibrium Molecular Dynamics," J. Chem. Phys. (to be published).

J. D. Johnson and J. C. Bonner, "Excitation Spectrum and Thermodynamic Properties of the Ising-Heisenberg Linear Ferromagnet," Phys. Rev. Lett. 44, 616 (1980).

J. D. Johnson and J. C. Bonner, "Excitation Spectrum and Low-Temperature Thermodynamics of the Ising-Heisenberg Linear Ferromagnet," Phys. Rev. B 22, 251 (1980).

J. D. Johnson, "A Survey of Analytic Results for the 1-D Heisenberg Magnets," J. Appl. Phys. 52, 1991 (1981).

J. D. Johnson, "A Comment on the Equation of State by Hirschfelder et al.," AIChE Journal 27, 166 (1981).

G. I. Kerley, "Perturbation Theory and the Thermodynamic Properties of Fluids. I. General Theory," J. Chem. Phys. 73, 469 (1980).

G. I. Kerley, "Perturbation Theory and the Thermodynamic Properties of Fluids. II. The CRIS Model," J. Chem. Phys. 73, 478 (1980).

G. I. Kerley, "Perturbation Theory and the Thermodynamic Properties of Fluids. III. Inverse-Power and 6-12 Potentials," J. Chem. Phys. 73, 487 (1980).

G. I. Kerley, "A Theoretical Equation of State for Methane," J. Appl. Phys. 51, 5368 (1980).

G. I. Kerley and J. Abdallah, Jr., "Theoretical Equations of State for Molecular Fluids: Nitrogen, Oxygen, and Carbon Monoxide," J. Chem. Phys. 73, 5337 (1980).

R. D. Dick and G. I. Kerley, "Shock Compression Data for Liquids. II. Condensed Hydrogen and Deuterium," J. Chem. Phys. 73, 5264 (1980).

D. A. Liberman, "Self-Consistent Field Model for Condensed Matter," Phys. Rev. B 20, 4981 (1979).

D. A. Liberman, "INFERNO: A Better Model of Atoms in Dense Plasmas," J. Quant. Spectrosc. Radiat. Transfer 27, 335 (1982).

G. K. Straub and B. L. Holian, "Thermalization Behavior Behind Shock Fronts in One-Dimensional Chains," Bull. Am. Phys. Soc. 24, 726 (1979).

G. K. Straub, B. L. Holian, and R. G. Petschek, "Molecular Dynamics of Shock Waves in One-Dimensional Chains. II. Thermalization," Phys. Rev. B 19, 4049 (1979).

C. E. Morris, J. N. Fritz, and G. K. Straub, "Shock Unloading and Reloading Profiles in Some Uranium Alloys to 15 GPa," Bull. Am. Phys. Soc. 24, 712 (1979).

G. K. Straub, B. L. Holian, and R. E. Swanson, "Molecular Dynamics of Shock Waves in Three-Dimensional Lennard-Jones Systems in the Solid Phase," Bull. Am. Phys. Soc. 25, 549 (1980).

R. E. Swanson, G. K. Straub, and B. L. Holian, "Molecular Dynamics of Sodium Using a Model Pseudopotential," Bull. Am. Phys. Soc. 26, 662 (1981).

G. K. Straub, R. E. Swanson, B. L. Holian, and D. C. Wallace, "The Thermal Properties of Metallic Sodium Near Melt from Molecular Dynamics Calculations," in the Proceedings of the CECAM Workshop on "Ab Initio Calculations of Phonon Spectra," Antwerpen, Belgium, edited by Devreese, Van Doren, and Van Camp (Plenum, 1982).

R. E. Swanson, G. K. Straub, and B. L. Holian, "Molecular Dynamics of Sodium Using a Model Pseudopotential," in the Proceedings of the 1981 Topical Conference on Shock Waves in Condensed Matter, Menlo Park, W. J. Nellis, L. Seaman, and R. A. Graham, Eds., (American Institute of Physics, New York, 1982).

R. E. Swanson, G. K. Straub, B. L. Holian, and D. C. Wallace, "Thermodynamic Properties of Solid Sodium from Quasiharmonic Lattice Dynamics and Molecular Dynamics," Phys. Rev. B 25, 7807 (1982).

D. C. Wallace and G. K. Straub, "Ensemble Corrections for the Molecular Dynamics Ensemble," Phys. Rev. A 27 (1983).

G. K. Straub, S. Schiferl, D. C. Wallace, and B. L. Holian, "Thermodynamic Properties of Fluid Sodium from Molecular Dynamics Calculations," (in preparation).

Reports

J. Abdallah, Jr., and W. F. Huebner, "QIKMIX: A Quick-Turnaround Computer Program for Computing Opacities of Mixtures," Los Alamos Scientific Laboratory report LA-7724-M (May 1979).

J. Abdallah, Jr., "MIXB: A BCON Controller for Generating and Maintaining Sesame Library Files of Mixture Data," Los Alamos Scientific Laboratory report LA-8219-M (April 1980).

J. Abdallah, Jr., G. I. Kerley, B. I. Bennett, J. D. Johnson, R. C. Albers, and W. F. Huebner, "HYDSES: A Subroutine Package for Using Sesame in Hydrodynamic Codes," Los Alamos Scientific Laboratory report LA-8209 (June 1980).

J. Abdallah, Jr., "Users Manual for CURVES," Los Alamos National Laboratory report LA-8844-M (October 1981).

R. C. Albers, "An Introduction to Two-Temperature Equations of State," Los Alamos Scientific Laboratory report LA-7934-MS (July 1979).

R. C. Albers and J. E. Gubernatis, "Brillouin-Zone Integration Schemes: An Efficiency Study for the Phonon Frequency Moments of the Harmonic, Solid, One-Component Plasma," Los Alamos National Laboratory report LA-8674-MS (January 1981).

B. I. Bennett, "Melting Under Shock Compression," Los Alamos Scientific Laboratory report LA-8567-MS (October 1980).

B. I. Bennett, "A Computationally Efficient Expression for the Zero-Temperature Isotherm in Equations of State," Los Alamos Scientific Laboratory report LA-8616-MS (December 1980).

B. I. Bennett, "EOSSCAN: A Program to Display Equation of State Data," Los Alamos National Laboratory report LA-8737-MS (March 1981).

Equation-of-State and Opacity Group (T-4 Group), "An Invitation to Participate in the LASL Equation of State Library," N. G. Cooper, Ed., Los Alamos Scientific Laboratory brochure LASL-79-62 (February 1980) and references therein.

F. Dowell and J. D. Johnson, "A Simple EOS for Polytetrafluoroethylene (Teflon)," Los Alamos National Laboratory report LA-9439-MS (August 1982).

F. Dowell, "A Simple EOS for Branched (Low-Density) Polyethylene," Los Alamos National Laboratory report LA-9559-MS (October 1982).

F. Dowell, "A Simple EOS for "Linear" (High-Density) Polyethylene (Marlex)," Los Alamos National Laboratory report LA-9564-MS (November 1982).

J. D. Johnson, "Electron Model for Gaseous UO_2 and the Effect on the UO_2 EOS," in "Nuclear Reactor Safety Quarterly Progress Report, April 1 - June 30, 1979," Los Alamos Scientific Laboratory report LA-7968-PR,NUREG/CR-0993 (August 1979).

J. D. Johnson and B. I. Bennett, "An EOS for Carbon Phenolic," Los Alamos National Laboratory report LA-9176-MS (March 1982).

J. D. Johnson and S. P. Lyon, "SES2D User's Manual," Los Alamos National Laboratory report LA-9164-M (April 1982).

E. H. Lieb and D. A. Liberman, "Numerical Calculation of the Thomas-Fermi-von Weizsäcker Function for an Infinite Atom without Electron Repulsion," Los Alamos National Laboratory report LA-9186-MS (April 1982).

G. I. Kerley, "A New Equation of State for Sodium," in "Nuclear Reactor Safety Quarterly Progress Report, April 1 - June 30, 1979," Los Alamos Scientific Laboratory report LA-7968-PR,NUREG/CR-0993 (August 1979).

G. I. Kerley and P. M. Henry, "Theoretical Equations of State for the Rare Gases," Los Alamos Scientific Laboratory report LA-8062 (January 1980).

G. I. Kerley, "User's Manual for Panda: A Computer Code for Calculating Equations of State," Los Alamos National Laboratory report LA-8833-M (November 1981).

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short summary for version   5 of sesame library file newmats
                  dated  12083 for  64 materials

number material              zbar  abar   r0 tables
  2290  lithium (z=3.0, a=6.  3.0   6.9   .5 101 201 301
  2982  molybdenum (z=42.00, 42.0  95.9 10.3 101 102 201 306
  3331  copper (z=29.00, a=6 29.0  63.5  8.9 101 102 201 301
  3712  aluminum (z=13.00, a 13.0  27.0  2.7 101 102 201 301
  5001  nitrogen (z=7.00, a=  7.0  14.0   .9 101 201 301
  5011  oxygen (z=8.00, a=15  8.0  16.0  1.3 101 201 301
  5171  argon (z=18.00, a=39 18.0  39.9  1.4 101 201 301
  5172  argon (z=18.0, a=39. 18.0  39.9  1.4 101 102 201 301
  5250  hydrogen (z=1.00, a=  1.0   1.0   .1 101 201 301
  5251  hydrogen (z=1.00, a=  1.0   1.0   .1 101 102 201 301 303 304
  5271  d-t mixture (z=1.00,  1.0   2.5   .2 101 102 201 301 303 304
  5411  neon (z=10.00, a=20. 10.0  20.2  1.2 101 201 301
  5502  methane (z=2.00, a=3  2.0   3.2   .5 101 201 301
  5520  ammonia (z=2.50, a=4  2.5   4.3   .7 101 201 301
  5762  helium (z=2.00, a=4.  2.0   4.0   .1 101 201 301
  7160  deutero-polyethylene  2.7   5.3  1.0 101 102 201 301 303 304 305
                                             306
  7171  polyethylene (branch  2.7   4.7   .9 101 201 301 303 304 305 306
  7180  polyethylene (marlex  2.7   4.7  1.0 101 201 301 303 304 305 306
  7190  teflon (polytetraflu  8.0  16.7  2.2 101 201 301 303 304 305 306
  7281  salt (z=14.0, a=29.2 14.0  29.2  2.2 101 102 201 301
  7371  lithium hydride (z=2  2.0   4.0   .8 101 102 201 301
  7541  carbon phenolic (z=4  4.6   9.0  1.5 101 102 201 301 303 304 305
                                             306
  7910  boron loaded silicon  4.9   9.6  1.8 101 102 201 301
  7920  cellular silicone ru  6.4  12.4  1.2 101 102 201 301
 12081  barium               56.0 137.3  3.5 101 201 501 502 503 504 505
 12100  praseodymium         59.0 140.9  6.8 101 201 501 502 503 504 505
 12110  europium             63.0 152.0  5.2 101 201 501 502 503 504 505
 12740  niobium              41.0  92.9  8.6 101 201 501 502 503 504 505
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38  12980  molybdenum              42.0   95.9 10.2 101 201 501 502 503 504 505
39  13120  cobalt                  27.0   58.9  8.7 101 201 501 502 503 504 505
40  13330  copper                  29.0   63.5  8.9 101 201 501 502 503 504 505
41  15030  dry air                  7.3   14.5   .0 101 201 501 502 504 505
42  15040  fluorine                 9.0   19.0  1.1 101 201 501 502 503 504 505
43  15050  bromine                 35.0   79.9  3.1 101 201 501 502 503 504 505
44  15180  krypton                 36.0   83.9  2.2 101 201 501 502 503 504 505
45  15190  xenon                   54.0  131.3  3.5 101 201 501 502 503 504 505
46  17080  boron carbide            5.2   10.7  2.5 101 201 501 502 504 505
47  17090  beb6                     4.9   10.1  2.3 101 201 501 502 504 505
48  17100  plastic bonded boron     4.6    9.2  2.0 101 201 501 502 504 505
49  17200  carbon tetrafluoride     8.4   17.6  2.0 101 201 501 502 504 505
50  17220  phosphorous trifluor    10.5   22.0  3.9 101 201 501 502 504 505
51  17240  lithium(6) deuteride     2.0    4.0   .8 101 201 501 502 504 505
52  17241  lithium(6) dt            2.0    4.3   .8 101 201 501 502 504 505
53  17560  polyurethane             3.8    7.0  1.3 101 201 501 502 504 505
54  17591  polystyrene+air          3.5    6.6   .1 101 201 501 502 504 505
55  17592  polystyrene+krypton      3.5    6.5  1.0 101 201 501 502 504 505
56  17600  epoxy                    4.6    9.0  1.2 101 201 501 502 504 505
57  17620  parylene (polymonoch     4.5    8.7  1.3 101 201 501 502 504 505
58  17830  carbon                   6.0   12.0  2.3 101 201 501 502 503 504 505
59  17840  boron nitride            6.0   12.2  2.1 101 201 501 502 504 505
60  22140  iron                    26.0   55.9  7.9 101 102 201 601 602 603
61  22700  gold                    79.0  197.0 19.3 101 102 201 601 602 603
62  22960  titanium                22.0   47.9  4.5 101 102 201 601 602 603
63  23100  nickel                  28.0   58.7  8.9 101 102 201 601 602 603
64  23200  lead                    82.0  207.2 11.3 101 102 201 601 602 603
65  23330  copper                  29.0   63.5  8.9 101 102 201 601 602 603
66  23540  tungsten                74.0  183.9 19.3 101 102 201 601 602 603
67  23710  aluminum                13.0   27.0  2.7 101 102 201 601 602 603
68  23810  silicon                 14.0   28.1  2.5 101 102 201 601 602 603
69  25010  oxygen                   8.0   16.0  1.3 101 102 201 601 602 603
70  25170  argon                   18.0   39.9  1.4 101 102 201 601 602 603
71  25260  deuterium                1.0    2.0   .2 101 102 201 601 602 603
72  25410  neon                    10.0   20.2  1.4 101 102 201 601 602 603
73  27830  carbon                   6.0   12.0  2.0 101 102 201 601 602 603
74
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notes.

tables 100-199  hollerith
tables 201      basic data
tables 301      total eos
tables 303      ion eos plus cold curve
tables 304      electron eos
tables 305      ion eos ( including zero point )
tables 306      cold curve ( no zero point )
tables 401      vaporization
tables 501      opacity grid check
tables 502      rosseland mean opacity
tables 503      electron conduction opacity
tables 504      mean ion charge
tables 505      planck mean opacity
tables 601      electrical conductivity
tables 602      electron conduction opacity
tables 603      mean ion charge



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7.0 Notre Dame Radiation Laboratory

7.1 Pulse Radiolysis Facility

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

   Answer: Reactive chemical intermediates produced by radiation are being examined on the nanosecond and longer time scale. These studies provide direct information on the importance of intermediates in chemical reactions which is not available by more conventional methods. Rates for the reactions of these intermediates are determined with high accuracy and are used to elucidate reaction mechanisms. New advances in computers and optical detection allow for significantly improved sensitivity and reliability of pulse radiolysis measurements. The rates and mechanistic data on radiation processes in solution are used in nuclear reactor design and are of importance in solar photochemistry research. Reactions of radicals within radiation tracks are of fundamental importance in nuclear medicine.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

   Answer: This linear accelerator-based pulse radiolysis facility is one of two in the U.S. actively carrying out studies of radiation-produced intermediates. Internationally there are about 15 pulse radiolysis facilities but none instrumented at the level of the NDRL facility or with similar capabilities. Certain features, such as the capability to do nanosecond pulse conductivity experiments, are completely unique worldwide. The high level of computerization of the data acquisition and processing systems makes it possible to support a wide variety of users and to employ procedures to examine details of reactions which are not available elsewhere.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

   Answer: A computerized system permits recording of optical data on radiation produced intermediates on the nanosecond and longer time scale. Signal averaging approaches are used to develop information not otherwise available in pulse radiolysis experiments. Because of the level of sophistication in data acquisition and processing this facility can be regarded as the most advanced of its type in the world.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

   Answer: Studies of acid-base neutralization by pulse radiolysis techniques show that the rate constant decreases with increased acidity and basicity. This finding challenges existing theories of the reactions of acids and bases and suggest that chemical relaxation can interfere with the high mobility of the proton. Reactions of OH radicals within radiation tracks have been explored using scavenging methods and it has been shown that about

50% of the OH initially produced reacts within 10 nanoseconds. It has also been possible to determine directly and accurately the rate constants of such reference reactions as for that between electrons and nitrous oxide in saturated solutions even though the reaction period is only 2.9 nanoseconds. Radiation chemical studies on photochemically produced excited states of porphyrins have recently been carried out and it has been shown that porphyrins are much more reactive in their triplet states than in the ground states available in nature. These observations are important in modelling photosynthetic processes. Currently studies are aimed at providing optical spectroscopic information needed for carrying out Raman experiments on radiation produced radicals. Studies are also in progress on the nature of the solvated electron in sodium hydroxide glasses and in very concentrated solutions of inorganic ions such as 14M lithium chloride where electrostatic effects can be important.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: The dedicated local microprocessor has recently been converted from a DEC PDP 8 to the more current DEC LSI11 technology. This allows reprogramming of on line data processing via FORTRAN routines rather than PDP 8 assembly language and more elaborate data treatment. A flash lamp pumped dye laser has been incorporated in the experiment so the pulse radiolysis studies on optically produced intermediates can be carried out. It is expected that the capability of this latter approach will be further exploited in the immediate future. An excimer pumped dye laser will be added to make this approach more versatile. Infrared equipment is expected to be added in the near future to allow reactions, particularly those of the hydrated electron, to be monitored in the 0.7 to 2.0 micron region.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer: Currently the annual operating budget is $65K. Associated research is $340K. Out-of-house research carried out by visiting scientists and collaboratively with staff of Laboratory. Capital equipment (8 MeV linear accelerator and associated equipment) is largely complete. An excimer pumped dye laser ($80K) is needed for the double pulse experiment. No specific construction projects are planned. Facility funds are provided by Chemical Sciences Division of the Office of Basic Energy Sciences.

(Budget Authority in Thousands)

	FY81	FY82	FY83	FY84	FY85
Facility Operation	50	50	55	60	70
In-House Research	190	210	230	240	250
Out-of House Research	60	70	80	100	120
Capital Equipment	35	10	25	50	80

7. How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?

Answer: No funding has been or is expected from other Federal agencies or private sources.

8. For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.

Answer: Staff levels are 2.5 man-years of technical support.

9. What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?

Answer: The facility has been operated on a 60-80 hours/week schedule for the past 5 years which is considered full utilization.

10. For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?

Answer: Approximately 300 projects have been supported during the past 5 years. Individual projects usually consist of a considerable number of related measurements made over a period of 2 to 6 months and integrated into a single overall objective (publication).

11. What is this facility's user policy?

Answer: The facility is open to external users for either independent or collaborative work. Collaboration of external users is encouraged.

12. For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?

Answer: None.

13. What is the mechanism by which specific research proposals for experiments at the facility are.considered?

Answer: Proposals should be submitted to the Laboratory Director after informal discussions with the staff as to experimental requirements and feasibility.

14. How many research proposals have been submitted over the past five years, and how many of these have been approved?

Answer: Approximately 300 projects have been submitted and approved for facility use. Experiments are considered only after feasibility has been established.

15. How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?

Answer: Approximately 45, including 15 faculty members, a number of Research Associates (Post Doctorals) and 5 Ph.D. candidates. A number of undergraduates from about 10 different universities have also participated in various aspects of these studies.

16. How many industrial researchers have utilized the facility over the past five years?

Answer: One industrial researcher has utilized the facility over the past five years.

17. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer: Twenty-five researchers from foreign institutions have utilized the facility over the past five years.

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: Two researchers from other agencies (Commerce, Agriculture) have utilized the facility over the past five years.

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: Equipment and minor facility improvements are made each year at the facility, however no major facility expansion is currently provided for in the budget. Future budgets and plans will of course consider improvements but right now no firm plans have been approved.

20. Please provide a copy of the facility's latest annual report.

Answer: Enclosed are Quarterly reports for the Laboratory Q-103--Q-106 covering 1983. [Note: Excerpts from these reports follow.]

956

NDRL 2454
(Q-103)

RADIATION LABORATORY

UNIVERSITY OF NOTRE DAME

QUARTERLY REPORT

January 1, 1983 - March 31, 1983

ISSUED

April 4, 1983

The Notre Dame Radiation Laboratory is a facility of the Department of Energy operated for DOE by the University of Notre Dame under contract No. DE-AC02-76ER00038. The majority of the programs within the Laboratory are supported by the Office of Basic Energy Sciences of DOE and, unless otherwise noted in the following, support can be attributed to the Office of Basic Energy Sciences. Certain additional programs, so indicated, are supported by DOE's Division of Environmental Research and Development and the Office of Standard Reference Data of the National Bureau of Standards.

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Mr. Thomas J. Dueweke, Mr. Edwin R. Hortelano and Mr. Michael F. Prebenda, undergraduate students at Kalamazoo College, spent the Kalamazoo winter quarter (Jan. 1 - March 31, 1983) with us working on their senior research problems. Mr. Dueweke carried out his research under the direction of Dr. L. K. Patterson, Mr. Hortelano with Dr. R. H. Schuler and Mr. Prebenda with Dr. D. M. Chipman.

Mrs. Marilyn K. Cagle joined the Laboratory's staff as secretary on March 28.

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Dr. P. V. Kamat of the University of Texas has accepted an appointment as an Assistant Professional Specialist and will join the staff in August. Dr. Kamat expects to initiate a program in the area of photoelectrochemistry.

Dr. Maria D. Pacheco of the University of Puerto Rico has accepted an appointment as Research Associate and expects to join the staff in July. She will be extending her studies on the ESR spectroscopy of photochemically produced radicals.

Dr. B. Venkataraman, Dean of Physics at the Tata Institute, Bombay, India, will spend the period May-August with us as a Visiting Research Associate.

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Dr. Peter Wardman of the Gray Laboratory, Mt. Vernon, England, visitied with us February 18-25. Dr. Wardman is collaborating with the Data Center on a compilation of one electron redox potentials of free radicals.

Publications

J. J. Kozak and O. E. Rossler
Weak Mixing in a Quantum System
Z. Naturforsch 37a, 33 (1982) [NDRL 2309]

J. P. Bays, S. T. Blumer, S. Baral-Tosh, D. Behar and P. Neta
Intramolecular Electron Transfer and Dehalogenation of Nitroaromatic Anion Radicals
J. Amer. Chem. Soc. 105, 320 (1983) [NDRL-2323]

R.M.P. Jaiswal, J. E. Katon and G.N.R. Tripathi
Infrared and Raman Spectra of Crystalline para-bromoaniline at Low Temperatures
Spectrochimica Acta 39A, 275 (1983) [NDRL-2328]

P. K. Das and G. L. Hug
Specific Hydrogen-Bonding Effects in the Photophysics of β-Apo-14'-carotenal. Static and Dynamic Aspects of Fluorescence and Triplet Yield Quenching
J. Phys. Chem. 87, 49 (1983) [NDRL 2338]

K. Miedlar and P. K. Das
Tris(2,2'-bipyridine)ruthenium(II)-Sensitized Photooxidation of Phenols. Environmental Effects on Electron Transfer Yields and Kinetics
J. Amer. Chem. Soc. 104, 7462 (1982) [NDRL 2339]

J. J. Kozak, M. K. Musho and M. D. Hatlee
Chaos, Periodic Chaos and the Random-Walk Problem
Phys. Rev. Letts. 49, 1801 (1982) [NDRL 2361]

J. J. Kozak, M. D. Hatlee, M. K. Musho, P. A. Politowicz and C. A. Walsh
Stochastic Flows, Reaction-Diffusion Processes, and Morphogenesis
J. Statistical Phys. 30, 263 (1983) [NDRL 2369]

I. Carmichael and K. Funabashi
Absorption Spectra of Dimer Negative Ions
J. Chem. Phys. 78, 23 (1983) [NDRL 2371]

R. Subramanian, L. K. Patterson and H. Levanon
Luminescence Behavior as a Probe for Phase Transitions and Excimer Formation in Liquid Crystals: Dodecylcyanobiphenyl
Chem. Phys. Letts 93, 578 (1982) [NDRL 2375]

B. Tembe and A. Mozumder
Electron Thermalization in Gases. V. Diatomic Molecules H_2, N_2 and CO
J. Chem. Phys. 78, 2030 (1983) [NDRL 2376]

M. Bazin, L. K. Patterson and R. Santus
Direct Observation of Monophotonic Photoionization in Tryptophan Excited by 300-nm Radiation. A Laser Photolysis Study
J. Phys. Chem. 87, 189 (1983) [NDRL 2378]

External Talks and Presentations

R. W. Fessenden
"Measurement of Dipole Moments of Photochemical Transients"
Brookhaven National Laboratories, Upton, NY, January 11, 1983
Argonne National Laboratory, Argonne, IL, March 31, 1983

NDRL 2492
(Q-104)

RADIATION LABORATORY
UNIVERSITY OF NOTRE DAME

QUARTERLY REPORT

April 1, 1983 - June 30, 1983

ISSUED
September 1, 1983

The Notre Dame Radiation Laboratory is a facility of the Department of Energy operated for DOE by the University of Notre Dame under contract No. DE-AC02-76ER00038. The majority of the programs within the Laboratory are supported by the Office of Basic Energy Sciences of DOE and, unless otherwise noted in the following, support can be attributed to the Office of Basic Energy Sciences. Certain additional programs, so indicated, are supported by DOE's Division of Environmental Research and Development and the Office of Standard Reference Data of the National Bureau of Standards.

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Dr. B. Venkataraman of the Tata Institute of Fundamental Research, Bombay, India, arrived on 5/16/83 to spend a three month period with us as a Visiting Research Associate.

Dr. Maria D. Pacheco of the University of Puerto Rico joined the staff on 6/28/83 as a Research Associate. She is currently carrying out studies on the photochemistry of inorganic complexes.

Dr. J. Phillip Bays of St. Mary's College joined the staff on a full time basis on 6/1/83 to spend the summer with us as a Visiting Research Associate.

Mrs. S. Venkataraman joined the staff of the Radiation Chemistry Data Center on 5/16/83 as a Research Specialist to assist with bibliographic surveys.

Miss K. Miller (6/1/83) and Mr. P. Lenoire (6/1/83) of the Chemistry Department have been appointed as Research Assistants. They are undertaking their Ph.D. studies under the direction of Dr. J. J. Kozak.

Gregory Erjavac and Farid Khairallah of the Electrical Engineering Department have been appointed as Research Assistants. They are undertaking their Ph.D. studies under the direction of Dr. E. Henry.

This year's summer student program includes Mr. T. Datta (Notre Dame, Department of Electrical Engineering - 6/1/83), Miss Y. Luo (Notre Dame, Department of Chemistry - 6/1/83), Mr. J. Barrera (Potsdam University - 5/23/83), Mr. H. F. Davis (Waterloo University - 5/1/83), Mr. C. Jinot (Waterloo University - 5/1/83), Mr. M. Hoptman (Michigan State University - 6/20/83), Mr. M. Wilson (Michigan State University - 6/20/83), Mr. S. C. Phan (Yale University - 5/16/83), Mr. R. King (Oberlin College - 6/1/83), Mr. S. Murphy (University of Colorado - 6/1/83), Mr. M. Prebenda (Kalamazoo College - 6/15/83), Mr. L. Qin (Shanghai University of Science and Technology - 6/16/83), Mr. R. Flint (Notre Dame, Department of Mathematics - 5/23/83) and Mr. D. Albright (Notre Dame, Freshman Year - 6/2/83).

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Dr. T. Wismontski has completed her appointment with us (4/30/83) and returned to the Weizmann Institute, Rehevot, Israel.

Dr. A. Vertes has completed his appointment with us (6/17/83) and returned to the Central Research Institute for Physics, Hungarian Academy of Sciences, Budapest, Hungary.

Dr. A. Gergely has completed her appointment with us (6/17/83) and returned to the Hungarian Academy of Sciences, Budapest, Hungary.

Dr. J. P. Mittal has completed his sabbatical year (4/30/83) and returned to the Bhabha Institute of Nuclear Research, Bombay, India.

Dr. L. Mittal has completed her appointment with us (4/30/83) and has returned to Atomic Energy College, Bombay, India.

Dr. P. Carton has completed his Ph.D. requirements under the direction of Dr. R. W. Fessenden and has returned to England.

Undergraduate students J. Considine (4/29/83), J. Federici (5/13/83), P. Wojda (5/2/83) and R. Vogt (5/13/83) have completed their studies and have left the staff.

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Dr. R. Davidson of Queens University, Kingston, Ontario, visited the Laboratory for the period 6/20-29/83 to continue his collaboration with Dr. J. J. Kozak.

Publications

J. M. Gould and D. H. Bell
Hydrogen Ion Permeability in Reconstituted Vesicle Systems
Chapter in Energy Coupling in Photosynthesis. Selman, Selman-Reimer, eds., Published by Elsevier North Haolland, Inc. p. 59 (1981) [NDRL 2254]

S. Muralidharan, G. Ferraudi, M. A. Green and K. G. Caulton
The Photochemistry of Rhenium Hydrides. A Flash Photolytic Investigation of the Transients in the Photochemistry of Tris(dimethylphenylphosphine)-pentahydridorhenium(V)
J. Organometallic Chem. 244, 47 (1983) [NDRL 2298]

D. M. Chipman
Theoretical Study of the Properties of Methyl Radical
J. Chem. Phys. 78, 3112 (1983) [NDRL 2354]

G. Ferraudi and S. Muralidharan
Photochemistry of Transition-Metal Phthalocyanines. Analysis of the Photochemical and Photophysical Properties of the Acido(phthalocyaninato)-rhodium(III) Complexes
Inorganic Chem. 22, 1369 (1983) [NDRL 2358]

S. Baral and P. Neta
Reduction and Alkylation of Cobalt(II) Tetrakis(4-sulfonatophenyl)prophyrin in Aqueous Solutions. A Kinetic Spectrophotometric Study
J. Phys. Chem. 87, 1502 (1983) [NDRL 2362]

O. Gonen and H. Levanon
EPR Study of Oriented Photoexcited Triplets of Zinc Porphyrin in a Discotic Liquid Crystal: Evidence for Axial Symmetry in the Condensed Phase
J. Chem. Phys. 78, 2214 (1983) [NDRL 2364]

G. Levey and T. W. Ebbesen
Methyl Viologen Radical Reactions with Several Oxidizing Agents
J. Phys. Chem. 87, 829 (1983) [NDRL 2370]

P. Umrigar, G. W. Griffin, B. A. Lindig, M. A. Fox, P. K. Das, T. M. Leslie, A. M. Trozzolo, S. N. Ege and A. Thomas
Generation and Characterization of Carbonyl Ylides from Pyrazolinone Spirooxiranes
J. of Photochem. 22, 71 (1983) [NDRL 2379]

D. M. Chipman
Comment on ab initio Calculation of Spin Densities in Hydrocarbon Radicals
J. Chem. Phys. 78, 4785 (1983) [NDRL 2382]

T. Wismontski-Knittel, I. Sofer and P. K. Das
Exciplex Processes Involving Trans Naphthylethylenes. Implications of Ground-State Conformeric Equilibria
J. Phys. Chem. 87, 1745 (1983) [NDRL 2383]

B. L. Tembe and A. Mozumder
Electron Thermalization in Gas Mixtures
Physical Review A 27, 3274 (1983) [NDRL 2403]

T. Wismontski-Knittel and T. Kilp
Effects of Aggregation on the Phosphorescence of Phenyl Alkyl Ketones in 77 K Rigid Glass Solutions
Chem. Phys. Letts. 96, 352 (1983) [NDRL 2405]

External Talks and Presentations

L. K. Patterson
"Photophysics in Spread Monolayers at the Air-Water Interface"
Kansas State University, Manhattan, Kansas, March 18, 1983

NDRL 2517
(Q-105)

RADIATION LABORATORY

UNIVERSITY OF NOTRE DAME

QUARTERLY REPORT

July 1, 1983 - September 30, 1983

ISSUED

February 21, 1984

The Notre Dame Radiation Laboratory is a facility of the Department of Energy operated for DOE by the University of Notre Dame under contract No. DE-AC02-76ER00038. The majority of the programs within the Laboratory are supported by the Office of Basic Energy Sciences of DOE and, unless otherwise noted in the following, support can be attributed to the Office of Basic Energy Sciences. Certain additional programs, so indicated, are supported by DOE's Division of Environmental Research and Development and the Office of Standard Reference Data of the National Bureau of Standards.

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Dr. H. Levanon of The Hebrew University, Israel, spent the period 7/1/83 to 8/31/83 with us as a Visiting Scientist.

Dr. C. Previtali of the faculty at Rio Cuarto University, Argentina, joined the staff as an Associate Professional Specialist while on leave from his university. He is working on various photochemical problems.

Dr. D. Geiger, a 1983 Notre Dame Ph.D., joined the staff on 8/1/83 as a Research Associate and is working on inorganic photochemical problems.

Dr. D. Mandell, Ph.D. Notre Dame 1979, joined the staff on 9/1/83 to assist with development of the Laboratory's computer systems.

Dr. P. V. Kamat, who received his Ph.D. from the University of Bombay, India, in 1978 and has held postdoctoral appointments at Boston University and the University of Texas, joined the staff on 8/1/83 as an Assistant Professional Specialist. He is extending his interests on photoelectrochemical problems.

Dr. Jay A. LaVerne, who has held a Research Associate appointment in the Laboratory, has been appointed as an Assistant Professional Specialist (9/1/83).

Dr. Paul Siders of California Institute of Technology (Ph.D. 1983) joined the staff on 7/5/83 as a Research Associate and is working on applications of statistical mechanics to solar energy problems.

Mr. O. Gonen, a graduate student at The Hebrew University, Israel, spent the period 7/7/83 to 9/15/83 with us as a special research student.

Mr. T. Dueweke, a 1983 B.S. graduate of Kalamazoo College, joined the staff as a Research Assistant and is assisting Dr. L. K. Patterson in studies of processes in monolayers.

Mr. E. Rivera of the Catholic University of Puerto Rico (7/21/83), Mr. L. Qin of Shanghai University of Science and Technology (6/16/83), and Mr. M. Ye of Peking Institute of Technology (8/9/83) have accepted graduate appointments in the Chemistry Department and research assistantships in the Radiation Laboratory.

Mr. M. Van De Putte (7/15/83) and Mr. R. Hibschman (8/8/83) joined the staff of the electronics shop.

Mr. D. Whitaker joined the Laboratory on 8/8/83 as machinist.

Mr. K. Houston, an undergraduate in the Electrical Engineering Department, joined the Laboratory as a Research Assistant on 9/28/83 and is assisting Dr. K. Madden with development of an ESR data acquisition system.

Dr. B. Venkataraman, on leave from the Tata Institute in Bombay, India, returned to his home institution on 8/31/83.

Dr. B. Tembe resigned from the Laboratory on 8/11/83 to accept an appointment at the University of Houston.

Dr. T. Kilp left the Laboratory on 8/31/83 to return to Canada.

Dr. F. Bayrakceken, on leave from Middle East Technical University, Ankara, Turkey, returned to his home institution on 8/31/83.

..rs. S. Venkataraman resigned her appointment with the Data Center on 7/11/83 to return to India.

Mr. M. Thomas resigned from the electronics shop as of 8/19/83 to continue electrical engineering studies at Purdue University.

Summer students R. Flint (8/5/83; Notre Dame), R. King (8/12/83; Oberlin College), J. Barrera (8/5/83; State University of New York at Potsdam), M. Prebenda (8/26/83; Kalamazoo College), M. Hoptman (9/9/83; Michigan State University), M. Wilson (9/16/83; Michigan State University), C. Jinot (9/2/83; University of Waterloo) and F. Davis (9/2/83; University of Waterloo) have returned to their respective universities.

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Dr. J. D. Hornak of Cornell University visited the Laboratory for the period 7/24-8/12/83 to continue his ESR studies in collaboration with Drs. Fessenden and Madden.

Dr. G. V. Buxton of Leeds University spent the period 9/5-17/83 working with the Radcation Chemistry Data Center.

Dr. R. Santus of the University of Paris spent the week of September 23 continuing his collaboration with Dr. L. K. Patterson.

Dr. Nianyun Liu of the Institute of Nuclear Research of Academia Sivica, Shanghai, China, spent the week of September 25 with us during his U.S. visit sponsored by tye Committee on Scholarly Communication with the People's Republic of China.

Publications

P. Natarajan and A. Radhakrishman
Photochemistry of cis-$[Co(en)_2(NO_2)_2]^+$ Ion in Acetonitrile
J. Chem. Soc., Dalton Trans. 12, 2403 (1982) [NDRL 2139]

R. Davidson and J. J. Kozak
Exact Dynamics of a Model for a Three-level Quantum System Interacting
with a Continuous Spectrum
J. Math. Phys. 27, 1911 (1983) [NDRL 2275]

R. H. Schuler and B. Behar
Scavenging Studies of OH Reactions within Radiation Tracks
Proceedings of The Fifth Tihany Symposium on Radiation Chemistry, Vol. 1,
p. 183 (1983) [NDRL 2318]

P. K. Das
Triplet-mediated Photoreduction of Viologens by Aromatic Hydrocarbons.
A Laser Flash-photolysis Study
J. Chem. Soc., Faraday Trans. 1, 79, 1135 (1983) [NDRL 2363]

R. M. P. Jaiswal, J. E. Katon and G. N. R. Tripathi
Polarized Infrared Spectra of Oriented Polycrystalline Films. Intermolecular
Vibrational Coupling in Crystalline 2,4,6-tribromoaniline
J. Chem. Phys. 79, 1 (1983) [NDRL 2365]

D. R. Prasad and G. Ferraudi
Electron-Transfer Quenching vs. Exciplex-Mediated Quenching of the
Low-Lying Excited States in Phthalocyanines
Inorganic Chem. 22, 1672 (1983) [NDRL 2368]

M. Bazin and T. W. Ebbesen
Distortions in Laser Flash Photolysis Absorption Measurements. The
Overlap Problem
Photochem. and Photobiol. 37, 675 (1983) [NDRL 2372]

D. E. Coyle, J. Bentley and D. H. Winicur
Energy Transfer Studies Between Ne* and H_2O
Chem. Phys. Letts. 97, 454 (1983) [NDRL 2389]

R. N. Sangster, K. P. Madden and R. H. Schuler
A Comparison of the Carbon-13 Hyperfine Constants of Carboxylated
Cyclohexadienyl and Hydroxycyclohexadienyl Radicals
J. Phys. Chem. 87, 2395 (1983) [NDRL 2391]

G. N. R. Tripathi and R. H. Schuler
Time-Resolved Resonance Raman Observation of Tetrafluoro-p-benzosemiquinone
Anion Radical
J. Phys. Chem. 87, 3101 (1983) [NDRL 2397]

C. V. Kumar, S. K. Chattopadhyay and P. K. Das
A Laser Flash Photolysis Study of Pyrene-1-Aldehyde. Intersystem Crossing
Efficiency, Photoreactivity and Triplet State Properties in Various Solvents
Photochem. and Photobiol. 38, 141 (1983) [NDRL 2398]

J. Granifo, G. Ferraudi and D. P. Rillema
Photochemistry of Copper(II) Macrocyclic Complexes: The Charge Transfer Photochemistry of 2,12-dimethyl-3,7,11,17-tetraazabicyclo[11,3,1]heptadeca-1(17),2,11,13,15-pentaenecopper(II)
J. of Photochem. 23, 51 (1983) [NDRL 2402]

D. Brault and P. Neta
Pulse Radiolysis of Porphyrin and Ferriporphyrin Solutions in 2-Propanol-Carbon Tetrachloride Systems. Protonation and Ligand Exchange Kinetics
J. Phys. Chem. 87, 3320 (1983) [NDRL 2404]

J. Grodkowski, P. Neta, B. W. Carlson and L. Miller
One-Electron Transfer Reactions of the Couple NAD·/NADH
J. Phys. Chem. 87, 3135 (1983) [NDRL 2411]

J. L. Hardwick
Determination of B-C for the (1,0,0) Vibrational State of Nitrogen Dioxide
J. of Molecular Spectroscopy 99, 239 (1983) [NDRL 2414]

S. K. Chattopadhyay, C. V. Kumar and P. K. Das
Triplet-related Photophysics of 9,10-diphenylanthracene. A Kinetic Study of Reversible Energy Transfer from Anthracene Triplet by Nanosecond Laser Flash Photolysis
Chem. Phys. Letts 98, 250 (1983) [NDRL 2415]

T. W. Ebbesen and M. Ohguchi
Methyl Viologen Aggregation
Photochem. and Photobiol. 38, 251 (1983) [NDRL 2420]

M. K. Musho and J. J. Kozak
Non-nearest Neighbor Random Walks in Reaction-diffusion Processes
J. Chem. Phys. 79, 1942 (1983) [NDRL 2427]

G. L. Jones, E. K. Lee and J. J. Kozak
Numerical and Analytical Studies of the Long-ranged Solutions of the Yvon-Born-Green Equation
J. Chem. Phys. 79, 459 (1983) [NDRL 2444]

C. V. Kumar, S. K. Chattopadhyay and P. K. Das
Triplet Excitation Transfer to Carotenoids from Biradical Intermediates in Norrish Type II Photoreactions of o-Alkyl-Substituted Aromatic Carbonyl Compounds
J. Amer. Chem. Soc. 105, 5143 (1983) [NDRL 2445]

G. N. R. Tripathi and R. H. Schuler
The Time-Resolved Resonance Raman Spectrum of Pulse Radiolytically Produced Phenoxyl Radical
Chem. Phys. Letts 98, 594 (1983) [NDRL 2451]

External Talks and Presentations

R. H. Schuler
"Pulse Radiolytic, Raman and ESR Studies of Transient Radicals"
Miller Conference on Radiation Chemistry, Hunfeld, West Germany, June 26, 1983

H. Levanon
"Triplet Dynamics in Anisotropic Media"
DuPont Experimental Station, Wilmington, Delaware, August 2, 1983

NDRL 2537
(Q-106)

RADIATION LABORATORY

UNIVERSITY OF NOTRE DAME

QUARTERLY REPORT

October 1, 1983 - December 31, 1983

ISSUED

February 23, 1984

The Notre Dame Radiation Laboratory is a facility of the Department of Energy operated for DOE by the University of Notre Dame under contract No. DE-AC02-76ER00038. The majority of the programs within the Laboratory are supported by the Office of Basic Energy Sciences of DOE and, unless otherwise noted in the following, support can be attributed to the Office of Basic Energy Sciences. Certain additional programs, so indicated, are supported by DOE's Division of Environmental Research and Development and the Office of Standard Reference Data of the National Bureau of Standards.

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Dr. M. V. George, a Visiting Professor in the Notre Dame Department of Chemistry and member of the faculty of the Indian Institute of Technology at Kanpur, India, joined the Laboratory staff on 10/1/83. Dr. George is continuing his interests in photochemical processes in organic systems.

Dr. Z. P. Zagorski of the Institute of Nuclear Studies, Warsaw, Poland, joined the staff as an Associate Professional Specialist on 11/21/84. Dr. Zagorski's interest in radiation chemical processes include current studies of electron decay in tert-butyl ammonium hydroxide clathrates.

Mr. M. Murphy, a graduate student at the University of Dublin, Ireland, spent the period 10/1/84-12/31/84 with us as a Research Assistant carrying out portions of his graduate thesis research.

Dr. S. Baral resigned from the Laboratory on 12/31/83 to accept an appointment at the Hahn-Meitner Institute.

Dr. H. Taniguchi, on leave from Yamaguchi University, returned to his university on 11/30/83.

Dr. J. Granifo resigned from the Laboratory on 12/31/83 to take up a faculty appointment at the University of Santiago, Chile.

Mrs. K. Flora resigned from the Data Center on 11/18/83 to accept a secretarial appointment with the ROTC.

Mr. R. Hibschman left the electronics shop of the Laboratory on 10/31/83 to accept other employment.

Mr. S. Knapik retired as Laboratory machinist on 12/31/83.

Publications

J. A. LaVerne and A. Mozumder
Penetration of Low-Energy Electrons in Water
Radiat. Res. 96, 219 (1983) [NDRL 2357]

G.N.R. Tripathi and R. H. Schuler
Time Resolved Raman Studies of Radiation Produced Radicals
Book "Time-Resolved Vibrational Spectroscopy" p. 199, Academic Press (1983)
[NDRL 2360]

M. Bazin and T. W. Ebbesen
Distortions in Laser Flash Photolysis Absorption Measurements. The Overlap Problem
Chemistry and Industry (Japanese Journal) 36, 816 (1983) [NDRL 2372]

S. Muralidharan and G. Ferraudi
Sequential Biphotonic Processes in Rhodium(III) Phthalocyanines
J. Phys. Chem. 87, 4877 (1983) [NDRL 2387]

T. Wismontski-Knittel and T. Kilp
Studies on the Role of Peroxy and Hydroperoxy Groups in Polymer Photodegradation
J. Polymer Science, 21, 3209 (1983) [NDRL 2400]

T. W. Ebbesen and G. Ferraudi
Photochemistry of Methyl Viologen in Aqueous and Methanolic Solutions
J. Phys. Chem. 87, 3717 (1983) [NDRL 2407]

J. D. Timpa, M. G. Legendre, G. W. Griffin and P. K. Das
Photoinduced Electron-Transfer Reactions of Aryl Glycosides
Carbohydrate Research 117, 69 (1983) [NDRL 2413]

H. A. Gillis and I. Carmichael
Bibliographies on Radiation Chrmistry: VIII. Radiation Chemistry of Crystalline Ice*
Radiat. Phys. Chem. 22, 981 (1983) [NDRL 2416]

S. K. Chattopadhyay, P. K. Das and G. L. Hug
Photoprocesses in Diphenylpolyenes. 2. Excited-State Interactions with Stable Free Radicals
J. Am. Chem. Soc. 105, 5205 (1983) [NDRL 2417]

A. Vertes
Quasifree Electron Mobility by the Method of Partial Waves in Liquid Hydrocarbons and in Fluid Argon
J. Chem. Phys. 79, 5558 (1983) [NDRL 2421]

E. Rivera and R. H. Schuler
Intermediates in the Reduction of 5-Halouracils by e_{aq}^{-1}
J. Phys. Chem. 87, 3966 (1983) [NDRL 2425]

G. R. Buettner, T. P. Doherty and L. K. Patterson
The Kinetics of the Reaction of Superoxide Radical with Fe(III) Complexes of EDTA, DETAPAC and HEDTA
FEBS 156, 143 (1983) [NDRL 2429]

R. M. P. Jaiswal, J. E. Katon and G. N. R. Tripathi
The Polarized Infrared Spectra and the Crystal Structure of 4,6-Dichloropyrimidine
J. Molecular Structure 102, 123 (1983) [NDRL 2431]

G.N.R. Tripathi
Time-Resolved Resonance Raman Spectroscopy of Radiation-Chemical Processes
ACS Symposium Series No. 236 "Multichannel Image Detectors" Vol. 2, 171 (1983) [NDRL 2433]

D. H. Winicur, J. L. Hardwick and S. N. Murphy
Spectroscopic Studies of the Helium-Acetylene Flame
Combustion and Flame 53, 93 (1983) [NDRL 2437]

J. L. Hardwick and W. J. Lafferty
High Values of ΔK_a in the Fluorescence of Nitrogen Dioxide and an Improved Fit of Ground State Inertial Constants
J. Molecular Spectroscopy 100, 358 (1983) [NDRL 2439]

A. Harriman, M. C. Richoux and P. Neta
Redox Chemistry of Metalloporphyrins in Aqueous Solution
J. Phys. Chem. 87, 4957 (1983) [NDRL 2461]

D. H. Bell, L. K. Patterson and J. M. Gould
Transmembrane pH Gradients and Functional Heterogeneity in Reconstituted Vesicle Systems
Biochim. Biophysica Acta 725, 368 (1983) [NDRL 2463]

R. H. Schuler, G.N.R. Tripathi, M. F. Prebenda and D. M. Chipman
Resonance Raman and Molecular Orbital Studies of the Effects of Deuteration on the Vibrational Structure of the p-Benzosemiquinone Radical Anion
J. Phys. Chem. 87, 5361 (1983) [NDRL 2468]

T. Nakayama
Site Selective Excitation of 1-Hydronaphthyl Radical in Irradiated Naphthalene Crystal
J. Luminescence 28, 313 (1983) [NDRL 2478]

H. F. Davis, P. K. Das, G. W. Griffin and J. D. Timpa
Mechanistic Aspects of 1,4-Dicyanonaphthalene-Sensitized Phototransformation of Aryl Glycopyranosides
J. Organic Chem. 48, 5256 (1983) [NDRL 2488]

B. L. Tembe, J. E. MacCarthy and J. J. Kozak
Transition Phenomena in Monolayers at the Air-Water Interface
J. Phys. Chem. 87, 4562 (1983) [NDRL 2501]

P. A. Politowicz and J. J. Kozak
Exact Algorithm for d-dimensional Walks on Finite and Infinite Lattices with Traps. III. Role of Lattice Valency in Influencing the Efficiency of Diffusion-Controlled Reactions
Phys. Rev. B 28, 5549 (1983) [NDRL 2504]

J. A. LaVerne and R. H. Schuler
Decomposition of Water by Very High Linear Energy Transfer Radiations
J. Phys. Chem. 87, 4564 (1983) [NDRL 2507]

G. Foldiak and R. H. Schuler
On the Reaction Mechanism of Scavenged Hydrocarbon Radiolysis
Z. Naturforsch 38a, 1154 (1983) [NDRL 2535]

*Supported by the Division of Environmental Research and Development and the Office of Standard Reference Data of the National Bureau of Standards.

External Talks and Presentations

R. H. Schuler
"Resonance Ramon Studies of Free Radicals"
Kalamazoo College, Kalamazoo, Michigan, October 18, 1983

7.2 Radiolysis-ESR Facility

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

   Answer: Free radicals produced by radiation are being directly examined by electron spin resonance (ESR) techniques in solution during irradiation with electron beams. The electron spin resonance facility provides for a combination of continuous, time-resolved and spin relaxation experiments unavailable elsewhere in the world. New advances in ESR spectroscopy make it possible to follow chemical reactions at times as short as nanoseconds. Chemical processes following absorption of high energy radiation are studied by identifying and defining the properties of the highly reactive radicals which are intermediates involved in the eventual production of chemical products. When it can be used, ESR unequivocally identifies the individual intermediates. Because of this specificity, the results obtained are very useful in connection with measurements by other methods, such as pulse radiolysis, and thus it is possible to obtain very detailed insight into the course of reactions involved in radiation processes. This fundamental information is important in the fields of photochemistry, general chemistry, radiobiology and reactor technology.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

   Answer: This facility is one of only two in the U.S. and three worldwide with the capability of carrying out electron spin resonance measurements during electron irradiation. The facility is completely unique in that continuous, time-resolved spin echo and spin relaxation studies can be carried out on radiation-produced transients in solution. Present computerization of the data acquisition system will give the facility additional, completely unique data processing capabilities.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

   Answer: Free radicals can be examined at nanosecond and longer times after preparation by electron beam techniques. Instrumentation is computerized at an advanced level for control of the experiment and for digital data acquisition and processing. As a result the sensitivity available is very high (10 E-7 M) so that radicals of very short lifetimes and containing carbon-13 at natural abundance levels can frequently be detected. Mechanistic and structural studies unavailable elsewhere can be carried out.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

   Answer: Spin exchange between hydrogen atoms has been shown to be important at distances of 10-20 Angstroms. This observation bears on considerations of interactions between molecular wave functions at large distances. ESR data have been obtained on carbon-13 containing radicals which permit electron distribution in oxygenated intermediates to be evaluated and provide information extremely valuable for theoretical studies of radical structure.

Recently, ionization of hydroxyl protons in hydroxycyclohexadienyl radicals has provided previously unavailable information on basicity scales for highly charged ions in very concentrated base (>1M). Studies in progress are aimed at extending structural and kinetic information of semiquinone radicals, important intermediates in naturally occurring electron transfer processes such as those prominent in photosynthesis.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: ESR equipment has been interfaced with the Laboratory's computer system via a local LSI11 microprocessor so that information can be stored and processed digitally. Currently spin-echo techniques are being added to the ESR apparatus to improve the time resolution available.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer: Currently the annual operating budget is $60K. Associated research is $320K. Out-of-house research is carried out by visiting scientists, largely collaboratively with staff of Laboratory. Capital Equipment (3 MeV Van de Graaff accelerator, ESR spectrometer and associated equipment) is largely complete. Recent acquisitions include a traveling wave amplifier for the spin echo experiment ($21K), transient recorder ($15K) and microprocessors ($10K) for computer interface. There have been no specific construction projects in the period. Facility funds are provided by Chemical Sciences Division of Office of Basic Energy Sciences.

(Budget Authority in Thousands)

	FY81	FY82	FY83	FY84	FY85
Facility Operation	45	52	56	60	68
In-House Research	200	225	240	250	275
Out-of house research	50	55	60	70	75
Capital Equipment	21	15	10	0	21

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer: No funding has been or is expected from other Federal agencies or private sources.

8. **For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.**

Answer: Staff levels are 2 man-years of technical support.

9. What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?

Answer: The facility has been fully used on a 40-50 hours/week schedule for the past 5 years. Experimental programs are expected to continue at least at this level in the immediate future. More extensive operation is limited by maintenance considerations.

10. For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?

Answer: Approximately 25 projects, each of which consists of many individual experiments, have been started or completed during the indicated period.

11. What is this facility's user policy?

Answer: The facility is open to external users for either independent or collaborative work. Collaboration of external users is encouraged.

12. For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?

Answer: None.

13. What is the mechanism by which specific research proposals for experiments at the facility are considered?

Answer: Proposals should be submitted to the Laboratory Director after informal discussions with the staff as to experimental requirements and feasibility.

14. How many research proposals have been submitted over the past five years, and how many of these have been approved?

Answer: Approximately 25 projects have been submitted and approved for facility use. Experiments are considered only after feasibility has been established.

15. How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?

Answer: Approximately 15, including 5 faculty members, 2 Ph.D. candidates, and 5 undergraduates.

16. How many industrial researchers have utilized the facility over the past five years?

Answer: None.

17. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer: Three researchers from foreign institutions have utilized the facility over the past five years.

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: One researcher from another agencies (Commerce) has utilized the facility over the past five years.

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: Equipment and minor facility improvements are made each year at the facility, however no major facility expansion is currently provided for in the budget. Future budgets and plans will of course consider improvements but right now no firm plans have been approved.

20. Please provide a copy of the facility's latest annual report.

Answer: Enclosed are Quarterly reports for the Laboratory Q-103--Q-106 covering 1983. (See answer to Question 20 concerning the Notre Dame Radiation Laboratory Pulse Radiolysis Facility in Section I.C.7.1 above.)

8.0 Oak Ridge National Laboratory

8.1 Electromagnetic Isotope Preparation Facility (Calutrons)

1. **What have been the facility's highlights for the period FY 1981 (or from start of operation if later than FY 1981) - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

   Answer: Operation of the Calutrons is an ongoing production routine. The enriched isotopes produced at the Electromagnetic Isotope Enrichment Facility are used in basic and applied research activities and in the production of radiopharmaceuticals for nuclear medical health-care delivery. Isotopically enriched materials are used in the determination of nuclear properties, in obtaining neutronic data for the design and operation of fission and fusion reactors, as tracers in analytical determinations, and as diagnostic tools in weapons testing. Their use in nuclear medicine includes biomedical research and as precursors for the production of diagnostic and therapeutic radioisotopes.

   The production of over three kilograms of thallium-203 over several year's time ending in FY 83, which is required for the preparation of the nuclear medical heart-scanning protocol thallium-201, has assured the uninterrupted supply of this important health-care agent.

   A new capability has been developed in FY 1983 whereby more than one multiisotopic chemical element can be enriched in a single, eight-separator magnetic segment simultaneously. While the quantity of each isotope separated in this manner is decreased per unit operating time, a greater variety of isotopes is produced to replenish the depleted inventory.

   The facility will interrupt separations during the last six months of FY 1984 due to a dip in sales revenue. However, chemical recovery and purification of a backlog of products will be accomplished during this period. We anticipate a return to the operation of two segments (16 separators) for FY 1985.

2. **What facility changes and additions have occurred or are anticipated for the period FY 1981 (or from start of operation if later) - FY 1985?**

   Answer: The present Electromagnetic Isotope Enrichment Facility is part of a facility originally constructed in the 1940's to provide enriched uranium for World War II atomic weapons. The utility systems have not been upgraded since the initial installation. Fiscal Year 1984 Accelerator and Reactor Improvements and Modifications (ARIM) funds will provide for the construction and installation of a new cooling tower needed for the magnet cooling system. The substantial increase in the capital equipment funds for FY's 83, 84, and 85 ($12M total) provide the ability to address the upgrade of the vacuum, coolant pumping, and electronic systems.

3. **For the period FY 1981 (or from start of operation) - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer: (Budget Authority in Thousands)

Item	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operations and Research	$2,400	$3,615	$3,275	$3,580	$5,000
BES - Nuclear Sciences	1,020	755	820	680	1,700
Isotope Sales Credits	1,380	2,860	2,205	2,500	2,700
NMA Stable Isotopes-ER	0	0	250	400	600
Out-of-House Research	0	0	0	0	0
Capital Equipment - BES-NES	48	32	200	500	500
General Plant Projects - MFE-ER	0	0	0	0	100
In-House Energy Management	0	0	0	0	0
Other Construction	0	0	0	270	0
TOTAL COST	$2,448	$3,647	$3,475	$4,350	$5,600

4. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer: No funds have been provided by other federal agencies, state agencies, foreign institutions, or private agencies.

5. **For the period FY 1981 (or from start of operation) - FY 1985, please provide actual and estimated staffing levels.**

Answer: The scientific and technical staffing levels are as follows:

	FY-81	FY-82	FY-83	FY-84	FY-85
FTE's	27.5	23.5	21.5	22.5	24.5

6. **What is the actual and estimated facility utilization for the period FY 1981 or from start of operation) - FY 1985? What would be defined as "full" utilization of the facility?**

Answer: Referring to the budget profile in the reply to question 3 of section 8.1, it is seen that utilization is dependent, to a significant degree, on the isotope sales credits. During the FY 81-83 period, an operating level of two segments (16 separator-years) has been maintained. In FY 84 this will decrease to two segments for 6 months, for a total of 8 separator-years. As previously discussed, this is due to the sharp drop in sales revenue experienced in FY 84. It is anticipated that a return to two-segment operation (16 separator-years) will be accomplished in FY 1985. It is estimated that an operational level of 22 separator-years per year is required to maintain equilibrium with current demand. The present operational capability is 30 separator-years per year.

7. **What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?**

Answer: The utilization of alternative enrichment technologies to supplement the existing Calutron capability by either "pre-enriching" the feed stock to allow enhanced throughput or direct substitution for specific isotope enrichment is considered a distinct possibility. A current study is directed toward an evaluation of the alternative methods and their applicability to the isotope enrichment program. At the conclusion of the task, appropriate plans and budget details will be developed.

8.2 EN-Tandem Facility

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

   Answer: Efforts here center on a better understanding of the interactions of energetic multiple-charged ions (MCI) with atoms, electrons and solids. Aside from the intrinsic importance of this work to atomic and solid state physics, the results contribute to plasma physics, astrophysics, and radiation physics as well as to associated technologies. By collinearly merging a space-charge-limited electron beam with an MCI beam we succeeded in measuring, for the first time, dielectronic recombination cross sections of MCI, an elusive but very important process in high temperature plasmas.

   Experiments at this facility were the first to show the dominance of multiple ionization in heavy ion-atom collisions and the essential failure of perturbation methods for handling these processes. Electron capture to the continuum (ECC) on MCI was first investigated here and showed that e.g., 1) ECC was a significant contribution to total charge transfer and 2) the shapes of ECC energy distributions give direct information about second-Born terms. Heavy ion channeling experiments were first performed at this facility and have since been highly developed to give information on the state of energetic ions penetrating solids, the interactions of MCI with solids, and the nature of the solids themselves. From the oscillatory motion of ions in channels we derive planar crystalline potentials; from precise energy losses of channeled MCI in "frozen" charge states we determine higher order terms in "electron gas" stopping power; from ionization of "frozen charged" ions as a function of velocity we observe "resonant coherent excitation" of ions which indicates the detailed ionic state, the nature of the crystal field and interactions of the ion's "wake" in the free electron sea.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

   Answer: The diversity of heavy ions available from the EN-Tandem Facility at ORNL is unequaled by any similar accelerator in the world. All ions lighter than neon have been provided to experimenters, and a wide variety of ions from magnesium to and including uranium have also been accelerated.

   A magnetically confined, space-charge-limited electron beam with a perveance of 10^{-6}, and a maximum energy of 3 keV is available for collinearly merging with a multiple-charged ion (MCI) beam. This unique capability has been used for making the only existing measurements of dielectronic recombination with MCI. The Elbek magnetic spectrograph has a mass-energy product of 100 and a resolution of 10^{-4}. These capabilities are unique among accelerator based atomic physics facilities. A beam line 20 meters long, equipped with two goniometers for channeling studies, is available, and has been used for heavy ion channeling measurements and for very small angle scattering studies. Incident beams may be charge state selected, and projectiles may be charge state analyzed after their interaction. Angular resolution of .002° has been achieved. The only MCI Penning trap has been used to make measurements of reaction rates of Ne^{q+} ions with various gases where the ion energies were in the range 1-10 eV and charge states ranged up to $q = 7$. Other devices and capabilities such as a very high resolution multichannel x-ray spectrometer, and an atomic hydrogen oven are unique in their availability in combination with a source of high energy multiple charged ions.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

Answer: 1) A magnetically-confined, space-charge-limited electron beam having a perveance of 10^{-6} and a maximum energy of 3 keV is available for merging with a heavy ion beam. This device has been used for the dielectronic recombination experiments. 2) An Elbek magnetic spectrograph having a mass energy product of 100 and an energy resolution of 10^{-4} is available. 3) Electrostatic and magnetic charge state analyzers are available. 4) A curved crystal x-ray spectrometer is used for the acquisition of cross section data, and satellite and hypersatellite spectra in the soft x-ray region. 5) A cylindrical mirror electron spectrometer with a resolving power of 500 can be used to measure Auger spectra from a differentially pumped gas target. 6) The data acquisition system based on a PDP 11/45 is being upgraded to a VAX based system. 7) A very high resolution (150 eV) Si(Li) detector is available. 8) A low energy positron generating station is under development. Currents of $\sim 10^5$ positrons/sec should be available. 9) A beam line, 20 meters long, is a available for channeling and small angle scattering experiments. Angular resolution is $\sim .002^{\circ}$. 10) A hydrogen depth profiling chamber is available. 11) A Rutherford backscattering target chamber is being developed.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer: 1) Dielectronic recombination cross sections were measured here for the first time. Results for B^{2+} and C^{3+} were published in 1983. This research will continue with other lithium-like ions O^{5+}, N^{4+}, and F^{6+}, and with neon-like ions such as Cl^{7+}, S^{6+}, and P^{5+}. 2) Investigations of electron spectra from projectile centered continuum states of heavy ions were initiated here. Examples of results are: (a) second-Born approximation asymmetry terms observed in electron spectra and (b) spectra and yields of convoy electrons from ions passing through solids and from channeled ions showed the contribution of ionization to the continuum cusps. Electron capture to continuum states by bare ions incident on atomic hydrogen will be investigated in 1984. 3) Channeling of heavy ions as a field of study, and as a tool for atomic and solid state physics was developed at this facility. Examples of results are: (a) experiments showed a strict $Z_1{}^2$ stopping power dependence of bare channeled ions and lack of higher order Z_1 effects; (b) resonant coherent excitation (RCE) of channeled ions was first observed on the ORNL EN-Tandem Facility; excitation of one and two electron ions in planar and axial channels was studied and the effect of oscillation amplitude on resonance strength was studied; and (c) Monte Carlo methods were used in 1983 to predict large enhancements of scattering at the "rainbow" angles for axially channeled ions. In 1984, experiments confirmed these predictions for protons passing through the <110> axial channel in silicon. In 1985 we will investigate the effect of rainbow scattering on RCE.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: During FY 1982 and FY 1983 an Elbek magnetic spectrograph was installed on an Accelerator Improvement and Modification project. The cost was $200,000. An Accelerator Improvement and Modification project is being carried out in FY 1984 and FY 1985 to upgrade the data acquisition system by the addition of a VAX CPU and various peripheral pieces of equipment. Cost for this upgrade will be $250,000.

6. For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).

Answer:

Budget Authority In Thousands

Item	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operations - BES Chem Sciences	$ 170	$ 170	$ 187	$ 235	$ 245
In-House Research - BES Chem Sciences	475	629	686	680	725
Other Operating Expense	0	0	0	0	0
Capital Equipment - BES Chem Sciences	23	55	85	90	100
AIP BES - Chem Sciences	200	0	0	250	0
General Plant Projects	0	0	0	0	0
In-House Energy Management	0	0	0	0	0
Other Construction	0	0	0	0	0
TOTAL	$ 868	$ 854	$ 958	$1,255	$1,070

7. How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?

Answer: The EN-Tandem has received no direct funding for operations from other Federal agencies, State agencies, foreign institutions, or private sources.

8. For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.

Answer: Staffing for the EN-Tandem Facility and for the related Accelerator Atomic Physics activity shown in person years, full-time equivalents is as follows:

		1981	1982	1983	1984	1985
EN-Tandem Operation:	Scientific	1.5	1.3	1.3	1.5	1.3
	Total Direct	1.8	1.6	1.6	1.9	1.7

		1981	1982	1983	1984	1985
Accelerator Atomic Physics:						
	Scientific	3.5	4.9	4.6	5.0	5.5
	Total Direct	4.1	5.8	5.9	5.7	6.1

9. What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?

Answer: We define full utilization of the EN-Tandem Facility to be two-eight hour shifts per day, seven days per week, with 75% of this time available for research and 25% used for maintenance. Utilizations are listed below for the fiscal years 1981-1985.

Fiscal Year	Hours	%
1981	1700	39
1982	2100	48
1983	1614	37
1984	2200	50
1985	2700	62

10. For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?

Answer:

Calendar Year	Started	Continued	Completed
1981	4	9	5
1982	5	8	2
1983	2	8	5
1984	5	10	5
1985	6	11	7

11. What is this facility's user policy?

Answer: The EN-Tandem Facility is open to qualified users from Oak Ridge National Laboratory, universities, and industries. Beam time and the use of existing devices and instrumentation are free of charge. Experiments are approved on the basis of a "request for beam time" by a Program Advisory Committee.

12. For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?

Answer: None.

13. What is the mechanism by which specific research proposals for experiments at the facility are considered?

Answer: The EN-Tandem Facility is open to qualified users from Oak Ridge National Laboratory, universities, and industries. Beam time and the use of existing devices and instrumentation are free of charge. Experiments are approved on the basis of a "request for beam time,'' by a Program Advisory Committee (PAC). The PAC consists of four staff members from the Accelerator Atomic Physics and EN-Tandem Operations groups. If the fractional utilization of the available time increases, and/or the number of requests from outside users rises, we will restructure the PAC to include outside user members. The only exception to the free beam time rule is for industrial users who request time for experiments that are not of direct interest to the Accelerator Atomic Physics Program. For these users a cost recovery charge has been made. In the last five years less than one week of time has been requested by one industrial user and the charges were less than $5,000.

14. How many research proposals have been submitted over the past five years, and how many of these have been approved?

Answer: Requests for beam time are generally requests for a block of one week of operation. Each additional week, for continuing experiments, requires a new request. Eighty-eight requests for beam time have been received over the last five years, and all have been approved.

15. How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?

Answer: Since January 1, 1979 there have been 35 faculty members, 29 students, and 20 postdocs, representing 26 different U.S. institutions, who have been users of the EN-Tandem Facility.

16. How many industrial researchers have utilized the facility over the past five years?

Answer: There have been two staff members from one company, Corning Glass, who have used the EN-Tandem Facility for profiling the depth distribution of hydrogen in leached glasses.

17. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer: Since January 1, 1979 there have been 17 faculty members, no students, 10 postdocs, representing 16 different foreign institutions, who have been users of the EN-Tandem Facility.

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: None.

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: The data acquisition system for the EN-Tandem Facility is being upgraded in FY 1984 and FY 1985. The existing data acquisition system is 15 years old and is built around a PDP 11/45 with limited peripherals and limited memory. The new system will be centered around a VAX 750 CPU, and will have terminals for collecting data in each of the three target rooms and terminals for accessing previously collected data from offices. Suitable peripherals are included. The total cost will be $250,000.

20. Please provide a copy of the facility's latest annual report.

Answer: The EN-Tandem Facility does not issue annual or progress reports but it contributes to the progress reports of the ORNL Physics Division. The last contribution to these progress reports is appended.

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PHYSICS DIVISION
PROGRESS REPORT
for Period Ending September 30, 1983

J. B. Ball, Director

Date Published: December 1983

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37831
operated by
UNION CARBIDE CORPORATION
for the
DEPARTMENT OF ENERGY

4. ACCELERATOR-BASED ATOMIC PHYSICS

The period covered by this progress report has been a time when a number of projects have been brought to fruition, and a number of new experiments have been completed or started. In this introduction we will give an outline of what is to follow, and the reader is referred to the individual contributions for details. We will also compare the status of each experiment to its corresponding status at the time of the last Physics Division Progress Report. At that time the merged heavy-ion electron beams experiment had been assembled but was not producing experimental results; the reasons for this failure were not understood, but possibilities were listed. In this chapter the first two results are reported. The reason for success now was not due td a single major advancement, but due to a great deal of effort to reduce each of the collection of experimental problems which initially plagued the effort. These first two results are reported in the first section on Ion Electron Collisions. In the last Physics Division Progress Report, it was noted that three atomic physics experiments for the Holifield accelerators had been approved by the Program Advisory Committee. All of these experiments on high energy charge transfer have been successfully performed, and their results are presented in the first, second, and fourth reports under Ion-Atom Collisions. The University of Tennessee experiments to measure electron capture and loss to projectile-centered continuum states have continued and have been supplemented by experiments to measure atom capture and loss to continuum states. The collaboration with North Texas State University on inner shell excitation has not been as active during this period as in prior periods. The analysis of the experiments on direct ionization of the target M shell, and target M shell to projectile K shell-electron transfer has been completed. Another Ion-Atom Collision contribution (the third contribution) is the result of collaboration between an ORNL staff member and the University of Aarhus, Denmark; thus collaboration is a two way street where we benefit not only by the stimulation from outside users coming to join our staff members and utilize our specialized facilities, but we also benefit by sharing our expertise with others. This premise is also illustrated by the last two contributions in the section on Lepton Solid Collisions.

Four other contributions to this chapter should be noted. The studies on collisional-, photo-, and auto-detachment electron spectroscopy on He$^-$ ions has been completed. With new funding, this collaborative effort between the Physics Division, the Health and Safety Research Division, and the University of Tennessee will be transferred to the Negative Ion Test Facility. There, they will be able to use a larger fraction of the facility time, and they will extend their studies to other negative ions. The University of Tennessee and Texas A and M collaboration has achieved their first results on charge exchange collisions of very slow (eV) highly charged heavy ions with molecules or atoms. These ions are produced as recoils from the passage of fast heavy ions through gases. The results are reported by C. S. O et al. The ion-ion collision experiment with the folded beam apparatus had not been conceived at the time of the last Physics Division Progress Report. Nevertheless, this one-man effort on a very difficult project is beginning to yield its first results as reported by H. J. Kim. Finally, one of our visitors from Boris Kidrič Institute has become entranced with the dynamics of ion channeling in very thin crystals. His predictions of the azimuthal and radial anisotropies of axial channeling patterns may be subject to experimental verification and his calculations may be relevant to some of the previously unexplained anomalies in resonant coherent excitation.

The installation of the Elbek magnetic spectrograph was completed during 1983. The use of this instrument will be inaugurated during the next year, probably initially for channeling experiments. We look forward to the installation of a new data acquisition system during the next two years. The specifications for this system are now being investigated. A new proposal on resonant coherent excitation has been submitted to the Program Advisory Committee of the Holifield accelerators. Undoubtably more proposals will be submitted for the next round of experiments.

In summary, a broad variety of accelerator based atomic physics experiments has been pursued during the period since the last report, and a broad program for the future is planned. The EN tandem supplemented by other facilities continues to be a forefront instrument for atomic physics research.

MEASUREMENT OF THE DIELECTRONIC RECOMBINATION CROSS-SECTIONS OF B^{2+} AND C^{3+} [1]

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The first measurements of the cross section for dielectronic recombination (DR) of multiply charged ions have recently been completed at the ORNL-EN tandem facility.[3] DR is the process by which electron capture from the continuum is facilitated via excitation of a previously bound electron followed by radiative stabilization. Using a merged electron-ion beam technique, we have measured the DR cross section of the lithium-like ions, B^{2+} and C^{3+}, where the resonant transition studied was

$$(1s^2,2s) + e^- \rightarrow (1s^2,2p,n\ell) \rightarrow (1s^2,2s,n\ell) + h\nu.$$

The merged beam apparatus is outlined in Fig. 4.1 The ion beam from the ORNL-EN tandem accelerator enters (through a 0.635 mm dia. hole in the cathode of the electron gun) a region, 84 cm long, in which the electron beam is magnetically confined. The doubly gridded Pierce-type high-intensity electron gun[4] is designed to produce a convergent, laminar electron beam. The beam comes to a focus ~7 mm from the anode where it has a diameter (containing 95% of the beam) of 3.15 mm. Magnetic confinement of the beam is accomplished by a coaxial solenoidal magnetic field adjusted to establish Brillouin flow.[5] Following the interaction region, the electrons expand due to space charge repulsion and strike the chamber walls while the ion beam is subjected to charge analysis through magnetic deflection. The initial charge state ion beam, A^{q+}, enters a Faraday cup and the ions that have picked up an electron, $A^{(q-1)+}$, are counted in a position sensitive particle detector (PSD). The A^{q+} current to the Faraday cup is fed into a current integrator and the output pulses are counted. The $A^{(q-1)+}$, ions arise from electron pickup due to charge transfer from residual gas molecules and slit edge scattering (the background) and DR (the signal). The overall length of the beam line is ~7 m and it is maintained at a pressure of $\sim 1 \times 10^{-9}$ Torr.

The experimental procedure consisted of optimizing the electron beam, at a particular cathode to anode voltage and counting the $A^{(q-1)+}$ and A^{q+} beams while stepping through the relative energies of interest by changing the energy of the ion beam. The deviation of the ratio, R, of (q-1)+ ions to q+ ions from a monotonic trend with ion beam energy gives a measurement of the DR cross section. The background ratio, R_B, can be fitted by a monotonic trend line ($\sim E_{ion}^{-2}$) and subtracted from R to yield the signal ratio, R_S. R_S is related to the DR cross section σ, by

$$R_S = \iint \rho_e \rho_i \, v_r \sigma \, dv_r \, d\Omega / \int \rho_i v_i \, dA$$

where ρ_e is the electron density, ρ_i is the ion density, v_r is the relative velocity, v_i is the ion velocity, and A and Ω are the area and volume of the interaction region, a cylinder whose radius is that of the ion beam r_i, and having the length of the electron beam, L; v_i is constant and the ion current I_i is given by $I_i = \pi r_i^2 \rho_i v_i$. Approximating ρ_e by an average electron density $\bar{\rho}_e$ times a distribution in relative velocities $f(v_r)$, both being independent of position within Ω, we can write that $R_S = (\bar{\rho}_e L/v_i)\langle v_r \sigma\rangle$, where the triangular brackets denote the average over $f(v_r)$. Defining an effective DR cross section, $\sigma_{eff} = \langle v_r \sigma\rangle / \langle v_r\rangle$, we then have $\sigma_{eff} = R_S v_i / (\bar{\rho}_e L \langle v_r\rangle)$.

To compare the derived experimental σ_{eff} with theoretical calculations[4] one must consider two details of the experiment in order to calculate an equivalent theoretical σ_{eff}. Since DR in both B^{2+} and C^{3+} leaves the resulting B^{1+} and C^{2+} in excited states dominated by high n states and since states above a maximum n $[n_{max} = 6.31 \times 10^{10} \, q^3/v_i B)^{1/4}]$ are field ionized by the charge analyzing field B, contributions to the theoretical σ_{eff} from states above n_{max} were deleted. Further, the experiment yielded a distribution in relative energy which was roughly Gaussian with a FWHM of 3 eV and this distribution was folded into the calculated σ to yield the theoretical σ_{eff}. The experimental values of σ_{eff} for B^{2+} and C^{3+} are listed in Table 4.1 and compared with predictions based on the Burgess-Merts theory (BM) and distorted wave calculations (DW). are shown in Table 4.1.

The quantitative agreement of our measurements with DW theory is quite good. The major experimental uncertainty affecting σ_{eff} is the determination of the electron density. The theoretical value is somewhat uncertain due to the effect of electric fields in the interaction region which tend to increase σ_{eff} above the zero field values shown in Table 4.1.

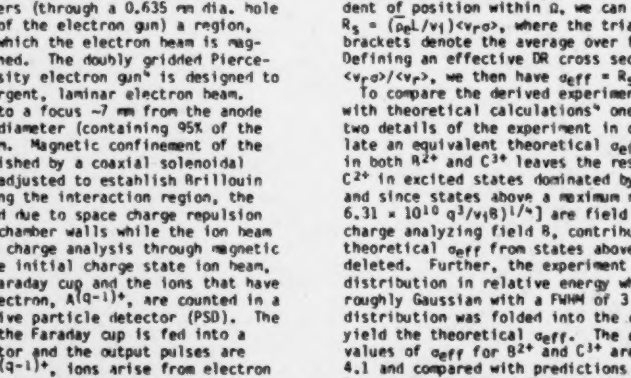

Fig. 4.1. Merged-beam apparatus.

Table 4.1. Theoretical and experimental DR effective peak cross-section values for B^{2+} and C^{3+} (ΔE_{rel} = 3 eV)

		σ_{eff}(10^{-19} cm^2		
Ion	n_{max}	BM	DW	Expt.
B_2+	22	2.6	1.1	1.0 ± 0.3
C_3+	26	4.0	1.6	2.1 ± 0.7

The experimental apparatus has recently been modified to decrease the background by decreasing the pathlength where charge transfer occurs. The charge analysis has been changed from magnetic to electrostatic and the geometry changed to allow smaller fields hence higher n_{max} and in turn larger σ_{eff}. It is hoped that these two modifications will lead to a fourfold increase in the signal-to-noise ratio.

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1. Summary of Paper: Phys. Rev. Lett. 51, 31 (1983).
2. On leave from Boris Kidrić Institute, Belgrade, Yugoslavia.
3. University of Delaware, Wilmington, DE.
4. Model 22-Ag-1, Hughes Aircraft Co., Electron Dynamics Division, Torrance, CA.
5. P. T. Kirstein, G. S. Kino, and W. E. Waters, "Space Charge Flow," McGraw-Hill Book Co., New York (1965), p. 153.
6. K. LaGattuta and Y. Hahn, Phys. Rev. A 26, 1125 (1982); D. McLaughlin and Y. Hahn, Phys. Rev. A 27, 1389 (1983); A. Burgess, Astrophys. J. 139, 776 (1964); R. D. Cowan, "The Theory of Atomic Structure and Spectra," Univ. of California Press, Berkeley, 1981; and A. L. Merts, R. D. Cowan, and N. H. Magee, Jr., Los Alamos Scientific Laboratory Report No. LA 6220-MS.

EXCITED STATE POPULATIONS AND CHARGE-EXCHANGE OF FAST IONS IN SOLIDS

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Excited state populations and charge state fractions of 36 MeV C and 445 MeV Cl ions have been measured for a range of thicknesses of gaseous and solid C targets. Cross sections for electron capture, loss, excitation and excited state quenching have been determined and these data are found to give a quantitative account of the Bohr-Lindhard density effect model. Implications of stopping power theory are considered.

Introduction

It is generally agreed that the density effect arises from the short inter-collision time in a solid relative to that in a low density gas. Two models, not mutually exclusive, have been proposed for the consequences of this short intercollision time, the Bohr-Lindhard[4] and Betz-Grodzins[5] models. In the former it is emphasized that excited states formed by electron capture or excitation are quenched by collisional ionization and thus lead to an apparent increase in the loss cross section and a decrease in the capture cross section relative to those in a gas target. Betz and Grodzins emphasized a model in which multiple vacancies with lifetimes in excess of the solid target transit time build up by collisions too rapid to allow projectile de-excitation; the projectile then changes charge after leaving the target by Auger emission.

A major physical simplification is achieved if one studies charge exchange of ions of sufficiently high velocity that the fully-stripped and hydrogen-like ion fractions dominate the charge-state distributions. Under these conditions Auger emission becomes negligible. We have investigated two such systems, 3 MeV/amu C and 12.7 MeV/amu Cl.

Method

Only a brief description of experimental methods is given here; the considerable amount of important detail in these procedures can be found in the report by Woods[6] and Moak et al.[7]

A single charge-state beam was passed through either a 1 m long differentially pumped gas target or a thin carbon foil. The emerging charge states produced by electron capture and loss in the target were spatially separated by electrostatic deflection and then counted with a P.S.D. This procedure was repeated for a range of target thicknesses and for incident fully stripped ions q = Z, H-like ions q = Z-1 and He-like ions q = Z-2. Nonequilibrium charge-state distribution data obtained for incident H-like ions on solid C targets is shown in Figs. 4.2 and 4.3 for C and Cl projectiles respectively.

The gas target data were obtained using 36 MeV C incident on C_2H_2, C_2H_4, C_2H_6, and CH_4; the target pressure covered the single collision linear growth regime and extended to the non-linear regime brought about by multiple collisions.

The H-like C^{5+} excited-state system was studied by carrying out beam-foil decay curve observations of Lyman series radiation using a grazing incidence grating spectrometer with entrance slits of 24 ± 1 μm to provide adequate spatial resolution. This spectrometer was carefully calibrated for detection efficiency-solid angle product and thus provided estimates of absolute photon yields. The spatial resolution was adequate to unravel the 3d-2p cascade, the only significant one, from the Ly_α decay curve and thus provided an estimate of both the 2p and 3d population at the foil exit. In addition the Ly_β decays were measured and provided the data to determine the 3p population. These observations were made for a range of carbon foil thickness down to about 5 atoms/$Å^2$. Equilibrium excited state populations and total equilibrium charge-state data are summarized in Table 4.2.

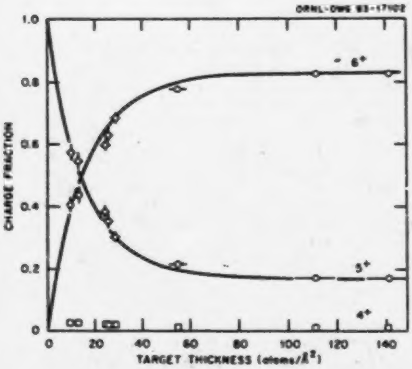

Fig. 4.2. Charge fraction emerging from C foils with C 5^+ incident versus foil thicknesses. The fits to the data used to determine the cross sections for electron capture and loss are also shown.

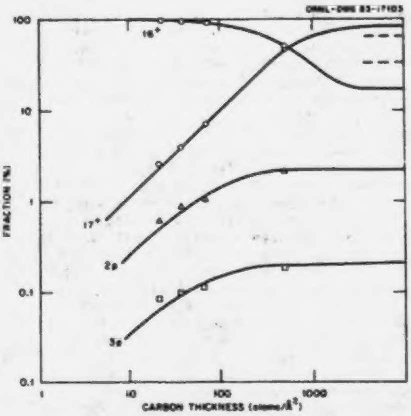

Fig. 4.3. Excited state and charge fractions from C foils versus foil thickness for Cl^{16+} ion incident. Also shown are the fits to the data using the cross sections of Table 3. The calculated gas target equilibrium values are indicated by dashed lines.

Table 4.2. Equilibrium Fractions (%) for 36 MeV C Ions.

Fraction	Solid C		Gaseous C	
*4+	0.80	± 0.08	1.4	± 0.1
*5+	16.6	± 0.5	25.0	± 0.5
6+	82.5	± 0.5	73.2	± 0.5
2s	0.30	± 0.04	0.31	± 0.04
2p	2.74	± 0.71		
3p	0.46	± 0.14		
3d	0.86	± 0.27		

*All states

The population of the $2s_{1/2}$ C^{5+} state was determined both for gaseous hydrocarbon targets and for thin C foils. This was done using a calibrated proportional counter placed to observe the Stark quenching of the 2s state via mixing with the 2p state and the consequent emission of Ly_{α} photons. The quench region was sufficiently downstream of the targets to provide only a small 2p natural decay background. Equilibrium values are shown in Table 4.2 for both gas and solid C targets.

The H-like Cl excited state fractions were obtained for a range of thin C foils by observing the total intensity of Ly_{α} transitions at the exit surface of the foil to a point downstream sufficient to observe decays from as high as about 16p. These measurements were carried out with a Si(Li) detector whose resolution including Doppler spread was about 150 eV. It was thus possible to resolve adequately Ly_{α} and Ly_{β} transitions at ~2.9 keV and 3.4 keV respectively. Other Lyman series lines out to the series limit could be detected but not resolved. The Si(Li) detector's efficiency was measured with an ^{55}Fe source at 6 keV and agreed with our calculated values. Observation of the intensity of Ly_{α} and Ly_{β} decays for a measured beam current served with the previously determined charge-state distribution data to calculate the excited state fractions. An example of these data is shown in Fig. 4.3 for Cl^{16+} incident on the foils. The spectroscopic data also indicated by the relatively low intensity of Lyman series lines from $n \geq 3$ that the only cascade of significance was likely to be the 3d-2p transition. Thus the estimated population for 2p includes the 3d population. Similarly the 3p population may contain a small cascade contribution.

Analysis and Cross-Section Results

The methods of analysis of nonequilibrium charge-state data in order to extract charge-exchange cross sections follows that discussed by Datz[8] and Betz-Grodzins.[5] A nonlinear least-squares fit was made to the charge fraction versus target thickness data for all the incident charge states by using the differential equations

$$\frac{d\phi_i}{dx} = \sum_{j \neq i} \left(\phi_j \sigma_{ji} - \phi_i \sigma_{ij}\right)$$

to generate values of the charge-state fractions using the cross-sections σ_{ij} for charge changing from charge i to charge j as free parameters. In the case of the 445-MeV Cl data the excited state fractions were treated as additional ϕ_i's. The errors on the data points used in the fitting routine included contributions from counting statistics and target thickness uncertainties.

Once cross sections had been obtained from the 36 MeV C data for each hydrocarbon gas their dependence on the number of H atoms per C atom in the molecule was used to extrapolate to free gaseous C values. In the case of electron capture and loss this was trivial as these were linear with the number of H atoms per C atom. The dependence of the $2s_{1/2}$ production and destruction cross sections on molecular environment was, however, not so simple and an arbitrary parabolic extrapolation was used to estimate the gaseous C cross-section values.

The various cross sections obtained from the nonequilibrium charge-state and $2s_{1/2}$ excited state populations is summarized in Table 4.3. Only charge-exchange between the dominant charge-state fractions of the equilibrium distribution are included.

The various electron capture and loss and excited state formation and destruction cross sections extracted by fitting the 445 MeV Cl data are given in Table 4.4.

Table 4.3. Cross Sections for 36 MeV C Ions (Units 10^{-3} $Å^2$/C Atom).

Process	Solid C	Gaseous C	Theory
$\sigma_{5,6}$	43.0 ± 3.0	27.0 ± 1.5	33.0
$\sigma_{6,5}$	8.0 ± 0.6	10.5 ± 0.5	10.4
$\sigma_{6,2s}$	0.65 ± 1.2	0.78 ± 0.03	1.4
$\sigma_{5,2s}$	0.92 ± 0.57	1.22 ± 0.08	
*σ_{2s}	228.0 ± 329.0	280.0 ± 10.0	246.0†
$\sigma_{5,2s+2p}$			15.0

*Destruction

†$\sigma_{2s,6} + \sigma_{2s,1s} + \sigma_{2s,2p} = 93.0 + 3.0 + 150.0$

Table 4.4. Cross Sections for 445 MeV Cl Ions (Units 10^{-3} $Å^2$/C Atom).

Process	Experiment	Theory
$\sigma_{16\to17}$	1.23 ± 0.03	1.8
$\sigma_{16(2p+3d)\to17}$	12.0 ± 9.0	7.2 to 16.0*
$\sigma_{16(3p)\to17}$	30.0 ±100.0	16.0
$\sigma_{17\to16}$†	0.61 ± 0.1	0.84
$\sigma_{17\to16(2p+3d)}$	0.28 ± 0.04	0.3, 0.05**
$\sigma_{16(1s)\to16(2p+3d)}$	0.28 ± 0.02	
$\sigma_{17\to16(3p)}$	0.06 ± 0.02	0.1
$\sigma_{16(1s)\to16(3p)}$	0.04 ± 0.01	
$\sigma_{16(2p+3d)\to16(1s)}$	0.0 ± 8.0	
$\sigma_{16(3p)\to16(1s)}$	0.0 ± 90.0	
$\sigma_{16(1s)\to16(2s,2p)}$		1.2
$\sigma_{16(1s)\to16(3s,3p,3d)}$		0.22

*Bohr n^2 scaling of $\sigma_{16(1s)}$ by 2^2 and 3^2

†All states

**$\sigma_{17\to2p}$, $\sigma_{17,3d}$

Discussion

Before examining the density effect for charge exchange in the two cases treated here, it is instructive to examine some theoretical predictions of the cross sections we have measured. Gillespie[9] has recently given Born approximation calculations of ionization and excitation of fast H-like ions colliding with He, N, and Ar. These values were scaled as $6^2/Z_t^2$, where Z_t is the appropriate He, N, or Ar nuclear charge. These estimates are included in Tables 4.3 and 4.4 where appropriate. The ionization cross sections for excited states was simply estimated by the Bohr[10] result

$$\sigma_{n\to\infty} = n^2\,\sigma_{1s\to\infty}.$$

Electron capture cross sections have been calculated using Eichler's[11] code for the Eickonal approximation. Capture was calculated separately for capture from the C target K shell and L shell. The Z_2 parameter of Eichler's calculations was chosen following Slater's rule. The electron screening parameter θ was calculated according to Eichler's prescription. The effective screened target charge Z_t^1 was chosen as 3.25 for capture from the target K shell and 1 for the capture from the target L shell so as to give good agreement between the 36 MeV C gas target total capture cross sections and the total capture cross section of the Eickonal approximation. The capture cross sections for 445 MeV Cl incident on C were made with the same choice of parameters as for 36-MeV C ions incident. The capture probability to different excited states is seen to be in reasonable accord with the data, Tables 4.3 and 4.4.

We see in Table 4.2 that 36 MeV carbon 4^+, 5^+, and 6^+ charge-state fractions are significantly different in gaseous and solid C targets. This density effect is thought to arise from the relatively large collisional ionization cross sections for excited states which have insufficient time to radiatively decay between successive collisions in a solid. In this context it is interesting to note that the metastable 2s population which does not radiatively decay between collisions even in the gas target at equilibrium pressures has virtually the same equilibrium population in the gas and solid. We therefore need to examine whether or not the excited state fractions 2p, etc., observed at equilibrium in solid C are sufficient to account for the observed density effect. It can be shown[12] that if one takes a single excited state approximation i.e. include only the 2p state, then

$$\sigma_{5,6}^{\text{solid}} = \sigma_{5,1s\to6} + n\,\sigma_{5,1s\to5,2p}$$

and

$$n = (\sigma_{5,2p\to6} - \sigma_{5,2s\to2p})/(\sigma_{5,2p\to6} + \sigma_{5,2p\to5,1s} + \sigma_{5,1s\to5,2p})$$

We obtain $\sigma_{5,1s\to6}$ from the gas target data Table 2 and use Bohr scaling to give $\sigma_{5,2p\to6} = 4\sigma_{5,1s\to6}$

$= 0.108 \text{Å}^2$/atom. De-excitation is found from Gillespie's theory: $3\sigma_{5,2p\to5,1s} = \sigma_{5,1s\to5,2p} = 0.015 \text{Å}^2$/atom to obtain $n = 0.63$ and hence $\sigma_{5,6}^{\text{solid}} = 0.037 \text{Å}^2$/atom. This compares to $\sigma_{5,6}^{\text{solid}} = 0.43 \pm 0.003 \text{Å}^2$/atom measured for 36 MeV C in solid C targets. Woods[6] has included the first few excited states in a more detailed model calculation and finds substantial agreement between the observed and calculated charge-state and excited state equilibrium fractions.

Turning now to examine the Cl data we see that the excited state collisional excitation and ionization cross sections which determine the density effect magnitude are obtained directly. It is thus a simple matter to predict both the solid and gas equilibrium charge-state distributions at least within the uncertainty of the poorly determined de-excitation cross sections. These values are shown in Fig. 4.3 and a substantial density effect is predicted. The gas target equilibrium values were estimated by setting the excited state ionization cross sections to zero and the de-excitation cross sections to infinity (large values). The predicted density effect is similar in magnitude to that observed for 36-MeV C in gaseous and solid C targets. We, therefore, conclude that the density effect model due to Bohr and Lindhard is substantiated in quantitative detail when reliable cross-section information is used.

Let us now turn to a consideration of the implications of these data to dE/dx predictions. It is commonly agreed that one may equate q_{eff} with the mean square charge in the target. In the cases studied here it is reasonable to equate q_{eff}^2 with q^2 the average squared charge calculated from the state distributions. The consequences of the density effect on q^2 between gas and solid targets for the fast ions studied here is easily shown to be only a few percent and hence only a small effect on the stopping power.[13] However, consideration of these individual electron capture, loss, excitation, and ionization processes for slower heavier ions whose charge-state distribution widths are broader than those of the nearly fully-stripped ions examined here presents a different picture. Betz[5] gives an expression for the change in mean charge Δq of a Gaussian charge-state distribution of e^{-1} width, $\Gamma = 2d_0\sqrt{2}$, when the single capture and loss cross sections determining the distribution are all changed by charge independent factors f_ℓ and f_c respectively i.e.

$$\Delta\bar{q} = d_0^2 \ \ln (f_\ell/f_c)$$

Taking values for f_ℓ and f_c of 1.68 and 0.8 as suggested by our C and Cl data gives $\Delta q = 0.69\, d_0^2$. Recently Pender and Hay[14] have studied 130-MeV Br in thin and thick C foils. If we accept their view that the thin foil charge-state data contain only a minor post-foil auger emission contribution to q we find $q = 21$ and $d_0 = 1.7$. Therefore, we predict a gas-solid charge-state difference of $\Delta q = 2.0$. Examination of the Br gas target data of Moak et al.[7] shows a gas, thin-C-solid Δq of 3.0. This implies a significant contribution to q_{eff}^2 in a solid relative to a gas and hence a significant difference between gas and solid stopping powers. The magnitude (20-40%) of such dE/dx differences for heavy ions in gas or solid targets observed by Geissel et al.[15] is in accord with the Δq estimate we make above.

Conclusion

The cross sections for electron capture, loss, excitation and excited state quenching have been determined for 3 MeV/amu C and 12.7 MeV/amu Cl. These data provide a quantitative description of the density effect for nearly fully-stripped systems. These observations are consistent with the emphasis placed on excited state ionization by the Bohr-Lindhard model. There is evidence to suggest that in partially stripped systems these same mechanisms also contribute significantly to the density effect.

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4. N. Bohr and J. Lindhard, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. 26, No. 12, (1954).
5. H. D. Betz, Rev. Mod. Phys. 44, 465-539 (1972).
6. C. J. Woods, D. Phil. Thesis, Oxford University, (1972).
7. C. D. Moak et al., Phys. Rev. 176, 427 (1968).
8. S. Datz et al., Phys. Rev. A2, 430 (1970).
9. G. H. Gillespie, Phys. Rev. A16, 943 (1977); Phys. Rev. A18, 1967 (1978); Phys. Rev. A22, 454 (1980).
10. N. Bohr, Kgh. DanskeVidenskab. Selskab., Mat.-Fys. Medd. 18, No. 8, (1948).
11. J.K.M. Eichler, Phys. Rev. A23, 498 (1981); J.K.M. Eichler and F. T. Chan, Phys. Rev. A20, 104 (1979).
12. N.E.B. Cowern, C. J. Woods, and C. J. Sofield, to be published in Nuclear Instruments Methods.
13. N.E.B. Cowern et al., Proceedings of the 10th International Conference on Atomic Collisions in Solids, July 18-22, 1983, Bad Iburg, F.R. Germany.
14. L. F. Pender and H. J. Hay, Phys. Rev. Lett. 24, 1970 (1983).
15. H. Geissel, Y. Laichter, W.F.W. Schneider, and P. Armbruster, Nucl. Instrum. Meth. 194, 21 (1982).

MEASUREMENTS OF SINGLE- AND DOUBLE-K-VACANCY X-RAY PRODUCTION CROSS SECTIONS OF TITANIUM FOR INCIDENT (Cl^{q+}) IONS AS A FUNCTION OF INCIDENT CHARGE STATE AND ENERGY

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K-X-ray-target production cross sections for Cl^{q+} ions incident on very thin titanium targets have been investigated in the incident particle energy range from 6.9 to 15.0 MeV/amu. This energy range corresponds to the transition velocity range $0.87 < v_1/v_{2K} < 1.3$, where v_1 is the incident projectile nuclear velocity, and v_{2K} is the mean velocity of an electron in the target K shell. For low projectile velocities and for v_1/v_{2K} sufficiently small, target K-vacancy-production is dominated by molecular orbital effects.[4] For sufficiently high velocities however, electron capture cross sections decrease, and both single- and double-K-vacancy-production-cross sections are dominated by direct ionization. This experiment was undertaken to investigate this transition region in the neighborhood of $v_1/v_{2K} \sim 1.0$ and with $Z_1/Z_2 \lessgtr 1.0$.

Cross sections for the production of titanium K_α-, K_β-X rays, and their respective hypersatellites were measured at five projectile energies between 6.88 and 15.05 MeV/amu. In each case the total cross section for the production of all K X rays, $\sigma_{KX}(T)$ was derived from the x-ray yield $Y_{KX}(T)$ using

$$Y_{KX}(T) = N_p\ \sigma_{KX}(T)\rho x\xi\Delta\Omega. \tag{1}$$

In Eq. (1) N_p is the number of incident projectiles, ρx is the areal atomic density of the target, measured by low energy proton backscattering, and $\xi\Delta\Omega$ is the Si(Li)-detector's solid angle, efficiency product. This latter factor was measured using a well calibrated ^{55}Fe source, and correcting the efficiency of the detector to the titanium x-ray energy. At each energy the charge-state distribution of chlorine ions exiting the target was measured in a separate experiment so that the number of incident particles could be derived from the measured charge integration of the transmitted beam.

At each energy, measurements were made with incident ions in charge states having more than two electrons, two electrons, one electron, and with bare incident ions. The two electron data will not be reported since the metastable fraction of the incident helium-like ions is not known. Each x-ray spectrum was fitted by a computer and the relative intensities of the K_α-, K_β-X ray, and their respective hypersatellites $K_\alpha{}^h$ and $K_\beta{}^h$ were extracted. The $K_\alpha{}^h$ cross section is then given in terms of the yields by

$$\sigma^h_{K\alpha} = \sigma_{KX}(T)[Y^h_{K\alpha}\ /\ Y_{KX}(T)]. \tag{2}$$

The total K-x-ray production cross section as a function of bombarding energy is shown for various incident projectile charge states in Fig. 4.4. The measurements at energies less than 5.0 MeV/amu were made at BNL, and have previously been reported.[4] Statistical error bars are shown for the data at 6.9 MeV/amu, and the statistical errors for the higher energy data are comparable. Systematic errors for the ORNL data bring the total error to ~ 30%. As anticipated, the cross section differences between different charge states decrease as the energy increases. We interpret this as a rather sharp decrease in the cross section for capturing at least one target K-electron by a projectile having one or more K vacancies when $v_1/v_{2K} \gtrsim 1$.

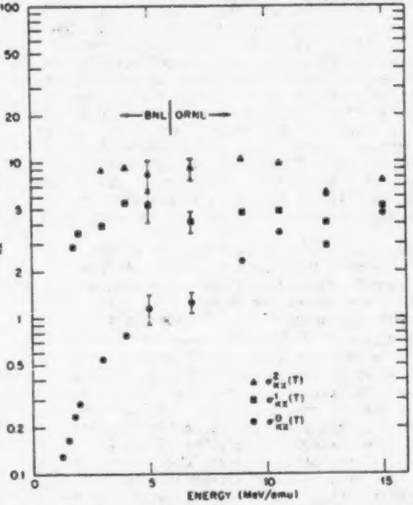

Fig. 4.4. Total K-x-ray-production cross sections for various Cl^{q+} ions incident on a vanishingly thin titanium target. The superscript on each of the cross sections, σ, is the number of K vacancies in the projectile. Data at energies below 6.0 MeV/amu were measured at BNL and have been previously reported (see Ref. 4); data at energies above 6.0 MeV/amu were measured using the Holifield coupled accelerators.

Figure 4.5 shows the ratio of $K_\alpha{}^h$, the hypersatellite yield, to the total K_α yield for various incident projectile charge states as a function of bombarding energy. Again the data at energies less than 5.0 MeV/amu are previously reported data measured at BNL, and the data at higher energies were measured using the Holifield coupled accelerators. Since many of the systematic errors affecting the absolute cross sections cancel in this ratio, the error

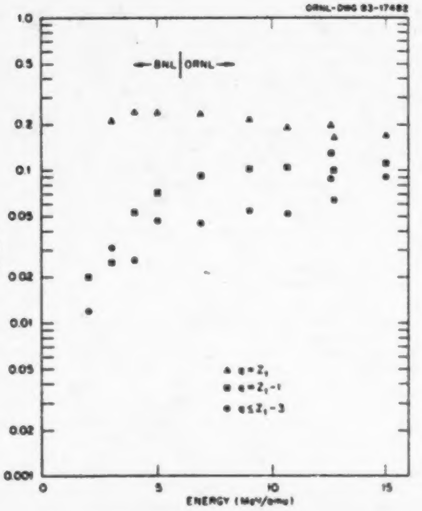

Fig. 4.5. The ratio of K_α^h, the hypersatellite yield to the total K_α-x-ray yield for various Cl^{q+} ions incident on a vanishingly thin titanium target. Data at energies below 6.0 MeV/amu were measured at BNL and have been previously reported (see Ref. 4); data at energies above 6.0 MeV/amu were measured using the Holifield coupled accelerators.

is dominated by the stripping procedure used to extract the hypersatellite yield. This error is estimated to be ~± 20%. It is certainly plausible to hypothesize from Fig. 4.5 that at sufficiently high energies double-K-shell vacancy production in the target will be dominated by direct projectile-double K-shell ionization.

The analysis of this data is continuing and comparisons to various theoretical models will be made before final publication.

TRANSFER IONIZATION AND TRANSFER WITH EXCITATION IN COLLISIONS OF 20 MeV Au^{q+} WITH HELIUM

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Measurements of forward directed electron spectra in coincidence with exit charge states in collisions of Au^{q+} (20 MeV) with He have disclosed two new phenomena which accompany charge transfer in the "medium" velocity (~2 v_0) region.

These experiments were intended to clarify some previous findings of the Aarhus group to wit: (1) In collisions of 20 MeV Au^{q+} with He they found that charge transfer occurs to high n states ($\bar{n} \approx q^{2/3}$) as anticipated from theory. (2) They measured partial cross sections, $\sigma_{q,q'}$ for the process:

$$\mathrm{Au}^{q+}(20\ \mathrm{MeV}) + \mathrm{He}^{0} \rightarrow \mathrm{Au}^{q'+} + \mathrm{He}^{n+} \quad (q = 5\rightarrow 24),$$

and observed large (~10^{-15} cm^2) cross sections for simple charge transfer, $\sigma^{0,1}_{q,q-1}$, and cross sections for double charge loss with only single capture, $\sigma^{0,2}_{q,q-1}$, which approached ~0.5 $\sigma^{01}_{q,q-1}$ in the region q = 14-24. They reasoned that the large values of $\sigma^{0,2}_{q,q-1}$ arose from the transfer of two electrons to excited states of the Au followed by autoionization. This process which has been dubbed "transfer ionization" is well established in the low energy ($v \lesssim v_0$) region. (3) Reasoning that the Auger electrons should be observable in the spectrum of electrons emitted from the rest frame of the moving gold ions (forward directed) they inserted an electrostatic analyser at 0° and measured electron spectra of the type shown in Fig. 4.6a for Au^{17+} and 4.7a for Au^{15+}. These showed a continuum peak (i.e., electrons moving at the same velocity as the Au ion beam) and subsidiary Auger peaks, electrons ejected from the Au with a few eV energy.

Although one might expect that the continuum electrons arose from capture to the continuum of these highly charged ions, the question arose as to the contribution of continuum states to "transfer ionization" i.e. the double loss from He occurring by the transfer of one electron to a bound state and of a second electron to the continuum. Accordingly we set up an experiment in which we measured the forward directed electron spectrum in coincidence with exit charge states q' = (q-1) and with q' = q, these being the only significant charge states emerging with q > 12 (note that if a coincidence is recorded with q-1 ion the product must be He^{2+}). The results shown in Fig. 4.6b and 4.7b are that (1) the continuum electrons are mostly coincident with Au ions which have also captured a bound electron and (2) the Auger electrons are not coincident with single capture by the Au (transfer ionization). They are coincident with Au ions that have not changed charge (transfer plus core excitation).

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[4] James Hall et al., Phys. Rev. A 28, 99 (1983), and references therein. See particularly Fig. 4.4.

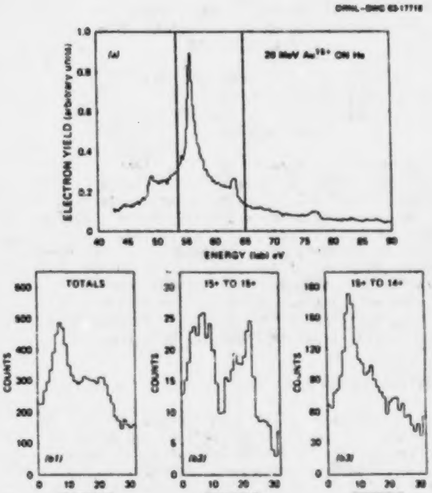

Fig. 4.6. a) Spectrum of forward directed electrons for 20 MeV Au^{15+} on He. b) Coincidence measurements in energy region delineated by vertical lines in a: b1 singles, b2 coincident with Au^{15+}, b3 coincident with 14^{+}.

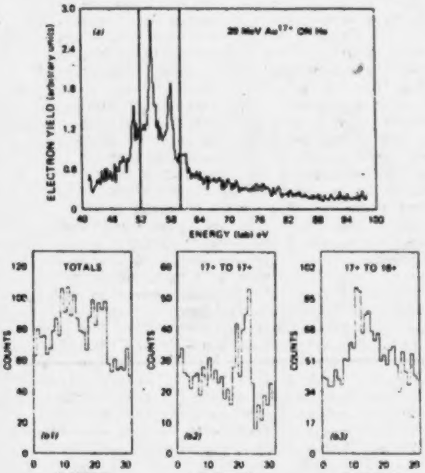

Fig. 4.7. a) Spectrum of forward directed electrons for 20 MeV Au^{17+} on He. b) Coincidence measurements in energy region delineated by vertical lines in a; b1 singles, b2 coincident with Au^{17+}, b3 coincident with Au^{16+}.

In another experiment we utilized a low charge state 20 MeV Au^{7+} beam, where $\sigma^{0,2}_{q,q-1}$ is small and no Auger electrons are observable, and measured electron spectra in coincidence with Au^{8+}. From the coincidence spectrum and a separate measurement of the absolute cross section for electron loss $\sigma_{7,8}$ we could establish (1) the correspondence between cross section and cusp electron yield and (2) the shape of an electron loss to continuum (ELC) peak. From the singles spectrum minus the 8+ coincidence spectrum we established the shape of an electron capture to continuum (ECC) peak (the shapes were in accord with measurements at other laboratories).

Using the information from the latter experiment we established for the collisions of the highly charged ions that: (a) the cross section for production of continuum electrons in coincidence with capture could account for the entire transfer ionization cross section and (b) the cusp shape was that for electron loss to the continuum (ELC) rather than ECC. This finding is in accord with the following simple model: at large distance an electron transfers from He into a high n state of Au; at a shorter distance the second electron transfers into a lower n state (higher ionization potential); during this second part of the collision the first electron is ionized to the continuum. The model, although simple, seems to describe the process well both qualitatively and semiquantitatively. The system studied, although it seems complex, is in fact simple since we are dealing with very highly charged particles ($q = 15\text{-}17+$) and hence high n hydrogenic states in interaction with a two-electron atom.

The process leading to Auger electron emission i.e., transfer plus core excitation emission has a large cross section ~2 x 10^{-17} cm^2 and is not as well understood. The cross section appears to be too large for noncorrelated events and may, in fact, be due to resonant transfer and excitation (RTE) which is related to dielectronic recombination and is much under discussion currently.

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ELECTRON CAPTURE TO THE CONTINUUM AT ASYMPTOTICALLY HIGH VELOCITIES

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A sharp cusp is observed in the ejected electron velocity spectrum in ion-atom collisions when the electron velocity $\vec{v}_e$ matches the emergent ion velocity $\vec{v}$ in both direction and speed. If the electron originates from excitation of a projectile electron to a low-lying continuum state, the process is termed electron loss to the continuum (ELC), and if a target electron is transferred to a low-lying (projectile) continuum state, the process is called electron capture to the continuum (ECC). If the projectile is bare only ECC can occur and the resulting cusp is asymmetric with higher intensity on the low-velocity side of the peak with the width observed to be roughly proportional to the ion velocity.[7] When several loosely bound electrons are available, ELC is the dominant process, producing a narrower, symmetric cusp peak.

To account for the ECC cusp shape asymmetry, Shakeshaft and Spruch[8] (SS) proposed inclusion of second Born expansion terms in calculation of the ECC cusp shape. In the second Born term all partial waves are thought to be important and an asymmetry results from odd-ℓ (p, f, ...) partial waves for which $d\sigma/dv$ is asymmetric under the formation $(\vec{v}_e - \vec{v}) + (\vec{v}_e - \vec{v})$. Their ECC cusp shape calculation for C^{6+} on H is characterized by a sheer drop in intensity on the high-velocity side of the peak. A modified first Born approach retaining terms linear in this difference has been proposed by Chan and Eichler[9] (CE). Because of an $\sim v^{-2\ell}$ partial wave dependence at asymptotically high velocities for first Born theories, the CE shape is dominanted by s partial-wave contributions and lacks the above-mentioned drop of the SS shape.

We present detailed results of recent measurements[10] of ECC for O, Ne, and Ar projectiles colliding with He at velocities 15-18 a.u. Using a partial-wave-expansion fitting method,[11] we find that for ECC at these velocities the p wave term gives a significant contribution to the cusp shape (Fig. 4.8), producing a drop in the ECC cross section for $v_e \gtrsim v$ qualitatively more similar to the SS shape than to the CE shape. However, the predicted strong projectile Z dependence of the asymmetry within the SS theory is not found for the projectiles studied here indicating a need for extension of the second Born calculations to helium targets.

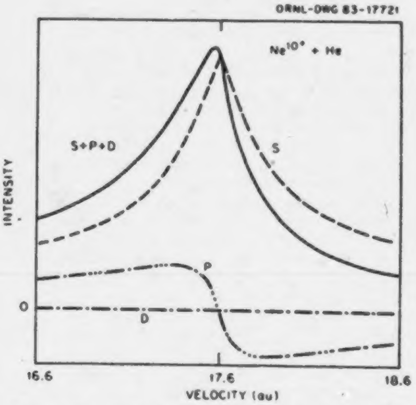

Fig. 4.8. Fitted ECC cusp shape (solid line) for 17.6 a.u. bare neon-He gas collision. Other curves are component partial waves of the fit.

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7. M. Breinig et al., Phys. Rev. A 25, 3015 (1982).
8. R. Shakeshaft and L. Spruch, Rev. Mod. Phys. 51, 369 (1979); Phys. Rev. Lett. 41, 1037 (1979).
9. F. T. Chan and J. Eichler, Phys. Rev. A 20, 367 (1979).
10. S. D. Berry et al., IEEE Transactions on Nuclear Science, NS-30, No. 2 (1983).
11. W. Meckbach, I. B. Nemirovsky, and C. R. Garibotti, Phys. Rev. A 24, 1793 (1981).

THE LINEWIDTH OF ELECTRON LOSS TO CONTINUUM CUSPS

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The velocity spectra of projectile electrons emitted in ionizing fast ion-atom collisions show a cusp at electron velocities $\vec{v}_e$ near the projectile velocity $\vec{v}_p$. This corresponds to an enhancement of the cross section for ionization to low-lying continuum states in the Coulomb field as seen in the rest frame of the projectile.

Recent experiments[4,5] focused on the shape of the electron loss to continuum (ELC) cusp as described by the linewidth (FWHM) of the singly differential cross section $d\sigma/dv_e$ (v_e) for electrons emitted within a narrow cone of half angle θ_0 around the forward direction. It is found that the ELC cusps are symmetric and narrow in comparison with electron capture to continuum (ECC) cusps.

We have initiated a systematic theoretical study of the ELC linewidth as a function of the initial bound state of the electron, its binding energy, the projectile velocity, and the target structure. Previous calculations for the ground state[6] are extended by evaluating the bound-free transition form factor $\langle \vec{k}^- | \exp(i\vec{q}\vec{r}) | n\ell m \rangle$ from arbitrary hydrogenic initial states $| n\ell m \rangle$ to low-lying continuum states $| \vec{k}^- \rangle$ with $k \ll (na)^{-1}$. This form factor determines the ELC cusp in Born approximation. The calculation can be done most conveniently by using an algebraic O(4,2) approach taking explicitly into account the dynamical symmetry of the Coulomb field. The result permits a systematic investigation of the angular distribution of the ejected electron.

In the rest frame of the projectile, the doubly differential cross section can be written as:

$$\frac{d\sigma}{d\vec{v}_e^{\,\prime}}(\vec{v}_e^{\,\prime}) = \sum_{\substack{k=0 \\ (k\ \text{even})}}^{2n} a_k(n\ell m)P_k^0(\cos\theta),$$

where $\cos\theta = \hat{v}_e^{\,\prime} \cdot \hat{v}_P$, and the coefficients a_k contain information about the initial state and the scattering dynamics. The highest-order anisotropy is determined by $k_{max} = 2n$ (not 2ℓ!). Therefore, the angular distribution becomes highly anisotropic with increasing principal quantum number n. Transformed into the laboratory frame, Eq. (1) leads to drastic changes of the ELC linewidth compared with Γ for an isotropic cusp (Fig. 4.9). In the calculation of $\Gamma(v_P)$, we have used hydrogenic wave functions with effective charges for the O^{5+} projectile.

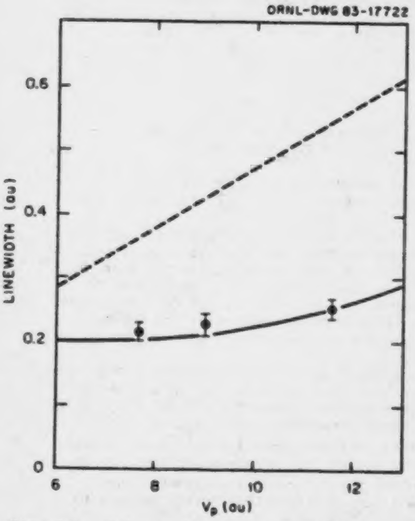

Fig. 4.9. ELC cusp linewidth Γ for O^{5+} on argon ($\theta_0 = 1.8°$). ——: present calculation; ----: Γ (vp) for isotropic electron emission; I: experimental data.

The argon target is treated in closure approximation. The resulting cusp shape is primarily determined by the loosely bound 2s electron yielding a narrow linewidth in agreement with the experimental data.

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4. M. Breinig et al., Phys. Rev. A 25, 3015 (1982).

5. R. Cranage, W. Steckelmacher, and M. Lucas, Nucl. Instrum. Meth. 194, 419 (1982).

6. J. Briggs and M. Day, J. Phys. B 13, 4797 (1980); and M. Day, J. Phys. B 13, L65 (1980).

ATOM CAPTURE AND ATOM LOSS AT ASYMPTOTICALLY HIGH SPEEDS

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P. Engar,[1]

Ion-atom collisions at asymptotically high speeds involving charge transfer or projectile or target ionization are the subject of many recent theoretical investigations. In the asymptotic velocity regime a perturbation expansion is supposed to provide an increasingly exact description of these processes. However, in current electron capture and loss experiments the asymptotic velocity regime can barely be reached. Furthermore, angular distribution measurements for charge transfer and projectile ionization processes become increasingly difficult at projectile speeds over 10 a.u. In experiments involving the capture of a whole atom from a molecule by a projectile ion or the loss of an atom from a projectile molecular ion, projectiles with kinetic energies on the order of 100 eV/u have asymptotically high speeds compared with characteristic vibrational speeds, while the laboratory scattering angles are measurably different from 0°. Doubly and triply differential cross section measurements become possible, thus revealing information about the scattering amplitudes.

For 200-300 eV/u Ar^+ and Kr^+ projectiles, we have measured the singly differential cross section $d\sigma/dv_H$ for capture of an H-atom from a CH_4 molecule into states lying in the vibrational continuum of the electronic ground state and into predissociative states of the projectile hydride molecule.[3] The proton yield into a cone of half-angle θ_0 about the beam direction exhibits a peak where the outgoing speed of the captured H-atom v_H equals the outgoing speed of the projectile ion v. Preliminary angular distribution measurements show that this peak is present only when $\theta_0 > \theta_c$, where θ_c is the critical angle for capture via the Thomas double scattering mechanism. Structure at equal velocity intervals above and below v arises from capture into predissociative states (see Fig. 4.10). For $\theta_0 = 1.6°$, $d\sigma/dv_H$ scales with projectile energy as $E^{-2.7}$ for Ar^+ projectiles and as $E^{-3.5}$ for Kr^+ projectiles.

In atom loss experiments, the shapes and yields of proton loss peaks were measured for 100-1300 eV/u H_2^+, HeH^+, ArH^+ molecular ions passing through various gas targets. Yields are only weakly dependent on the target gas and increase with projectile energy. Shapes

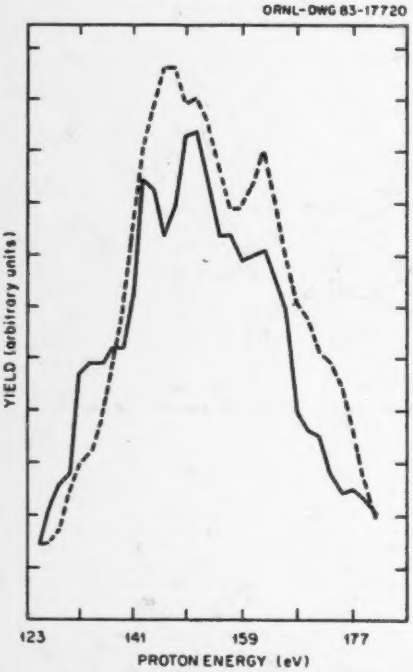

Fig. 4.10. Energy spectra of protons into a cone of half angle $\theta_0 = 1.6°$ (broken line) and $\theta_0 = 2.6°$ (solid line) centered about the beam direction after capture by 6.06 keV Ar^+ projectiles on CH_4. A linear background has been subtracted.

and width are independent of projectile and target. For projectile energies above ~175 eV/u, prominent features in the wings of the proton loss peaks indicate excitation of dissociative states of the projectile molecule. The positions of these features are independent of projectile velocity or target gas, but the production cross sections are strongly energy- and target-dependent.

COLLISIONAL- AND AUTO-ELECTRON DETACHMENT SPECTROSCOPY OF NEGATIVE IONS

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D. J. Pegg[2]

A considerable amount of effort has been expended by several research groups toward illucidation of the complex physical processes of electron capture (ECC) and loss (ELC) to energetic projectile centered continuum states which occur as a consequence of their traversal through thin solid and gaseous targets. Many of the studies have involved the use of multiply charged heavy positive ions at a few to several MeV in energy. However, recent studies have been made of the ELC processes accompanying interactions between negative ions and thin gaseous targets at low energies.

Duncan and Menendez[3,4] have utilized H^- projectiles in measuring ELC differential cross sections in energy and angle resulting from interactions with thin noble gas targets at projectile energies between 0.5 and 1 MeV. As a consequence of these investigations, discovery was made of target dependent structures in the ELC energy spectra near $\theta \approx 0°$ from both He and Ar targets. These discoveries have evoked considerable theoretical interest concerning the underlying mechanisms responsible for these phenomena. Theoretical studies have been made of the ELC processes resulting from H^- projectile interactions with He and Ar by Maleki and Macek,[5] Crawford[6] and more recently by Burgerdörfer.[7] The double peaked structures have been shown to be a consequence of destructive interference between the $\ell = 0$ and higher order $\ell > 0$ partial waves.

As a continuation of the previously reported investigation of the lifetime and eigenenergy determination of the metastably bound states of He^-,[8] we have measured ELC energy spectra near $\theta = 0°$ for H^- and He^- projectiles interacting with a variety of thin gaseous targets at projectile energies between 20 and 120 keV. The experimental apparatus utilized in these investigations has been previously described[8] and therefore will not be reported in this article. No reproducible structures were observed in the resulting H^- ELC electron energy spectra from thin He and Ar targets which could be correlated with the interference phenomena discovered by Menendez and Duncan. Examples of the background subtracted ELC spectra from H^- and He^- interaction with argon at various projectile energies are shown respectively in Figs. 4.11 and 4.12. As noted, the ELC spectra for each of the projectiles are slightly skewed toward higher projectile velocities. The spectra for H^- are found to be remarkably cusp-like in shape in spite of the dominance of single electron loss processes (SEL). This is rather surprising since the final state projectile-electron interaction cannot be described in terms of cusp producing Coulomb wave functions. On the other hand, the spectra from He^- is not cusp-like even though the double electron loss process for He^- is expected to dominate due to the ease of removal of the two excited electrons present in the $^4p°$ He^- configuration.

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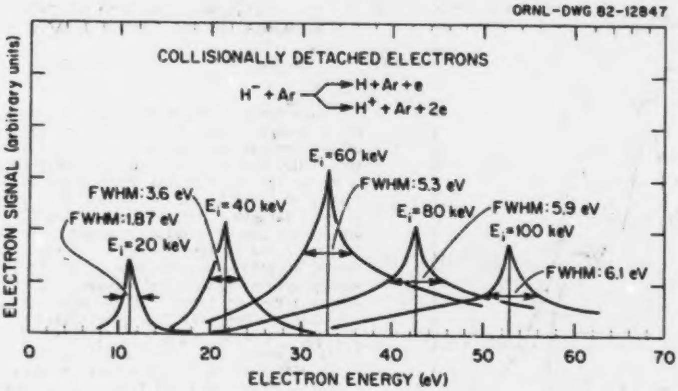

Fig. 4.11. Collisionally induced projectile electron loss energy spectra for H^- incident on thin argon targets.

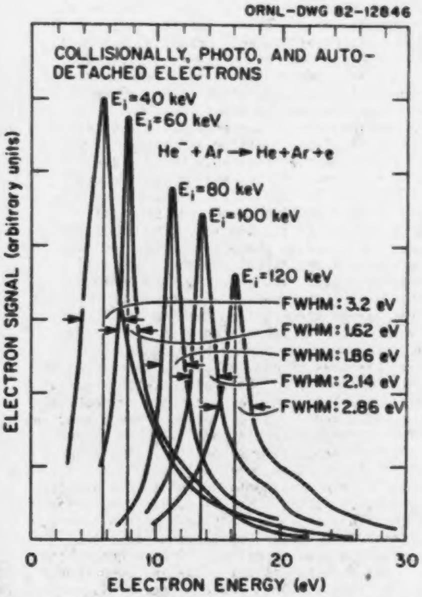

Fig. 4.12. Collisionally induced projectile electron loss energy (ELC) spectra for He^- incident on thin argon targets.

An anomonously large (ELC) peak centered at $v_e = v_i$ is found for He^- which is present at the lowest attainable pressures (~ 1×10^{-7} torr in our experimental apparatus) indicating the presence of another mode of decay other than through collisional processes. Efforts are underway to try to explain this effect. An example of one such attempt is shown in Fig. 4.13 where it is clearly shown by use of a simple heat lamp that black hody photo-detachment processes may contribute to the pressure independent peak. Experiments such as those described above are continuing with emphasis on determination of the properties of metastably bound negative ion states. Specifically, two projects are underway which will permit determination for the first time of the lifetimes and eigenenergies of metastable ions such as Be^- and Ca^-. In order to measure and detect very short half life states, we have designed and constructed a new experimental apparatus which is closecoupled to the region of ion generation. This experimental arrangement should permit measurement of lifetimes <1 μsec.

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1. Health and Safety Research Division.
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3. M. M. Duncan and M. G. Menendez, Phys. Rev. A 16, 1799 (1977).
4. M. G. Menendez and M. M. Duncan, Phys. Rev. A 20, 2327 (1979).
5. N. Maleki and J. Macek, Phys. Rev. A 26, 3198 (1982).
6. O. Crawford (to be published).
7. J. Burgerdörfer, Phys. Rev. Lett. 51, 374 (1983).
8. G. D. Alton, R. N. Compton, and D. J. Pegg, Phys. Rev. A 28, 1405 (1983).

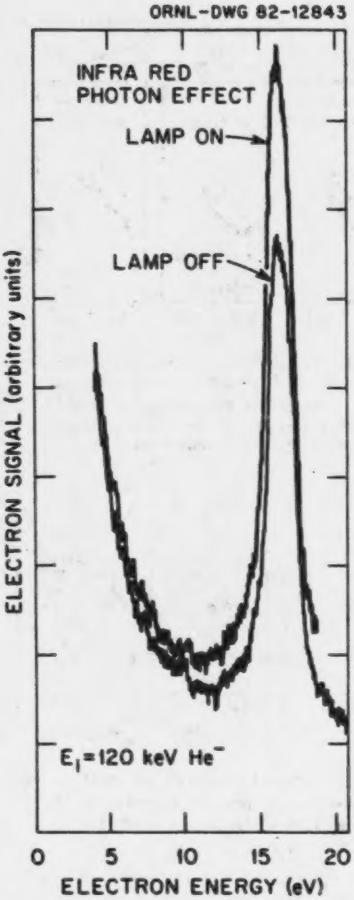

Fig. 4.13. Illustration of pressure independent ELC electron spectra from He⁻ and the infrared photo detachment effect.

DIRECT IONIZATION AND ELECTRON CAPTURE IN M-SHELL X-RAY PRODUCTION BY FLOURINE IONS[1]

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G. Lapacki[4]
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A. R. Zander[6]

Direct ionization to the target continuum (DI) and electron capture to the projectile (EC) are the primary mechanisms involved in inner-shell vacancy production in heavy-ion-atom collisions. Two theoretical methods used in the present work to understand these processes are the first Born approximation and the ECPSSR (energy loss, Coulomb deflection, perturbed stationary state, with relativistic effects) method. In the first Born approach, the contribution of DI is calculated in the plane-wave-Born approximation (PWBA)[7] and the contribution of EC is calculated in the Oppenheimer-Brinkman-Kramers (OBK) approximation of Nikolaev (OBKN).[8] The ECPSSR approach,[9] based on the perturbed-stationary state (PSS) formalism,[10] goes beyond the first Born approximation and takes into account energy loss, Coulomb deflection, and relativistic effects. The ECPSSR has recently been extended by Lapicki[11] to M-shell ionization.

Studies by McDaniel and co-workers for K-shell ionization by $^{28}_{14}$Si ions[12] and for L-shell ionization by $^{19}_{9}$F, $^{28}_{14}$Si, and $^{35}_{17}$Cl ions[13] found enhancements in the cross sections for projectiles with K-shell vacancies over those without K-shell vacancies. This enhancement was successfully explained by the EC theory of Lapicki and McDaniel,[14] based on the perturbed-stationary-state approach. The present work was undertaken to broaden the scope of these measurements to M-shell ionization and to make comparisons with currently available theories.

M-shell x-ray production for vanishing thin targets of $_{79}$Au, $_{82}$Pb, $_{83}$Bi, and $_{92}$U were measured for 25-, 27-, and 35-MeV $^{19}_{9}F^{q+}$ ions. The charge states of the fluorine ions ranged from q = 6,8,9 at 35 MeV to q = 4,5,6,8,9 at 25 and 27 MeV. The M-shell x-ray production cross sections for projectiles with one or two K-shell vacancies are compared to the average M-shell x-ray production cross sections for projectiles without K-shell vacancies. Cross sections for DI plus EC to L,M,... shells and EC to the K shell of the projectile are inferred and compared to the predictions of the first Born and ECPSSR theories.

The 25-, 27-, and 35-MeV $^{19}_{9}F^{q+}$ ions were produced by the EN Tandem Van de Graaff accelerator. The ion beam was magnetically selected for charge states q = 4,5,6,8, or 9 at 25 and 27 MeV and q = 6,8, or 9 at 35 MeV. After collimation, the ion beam was incident on targets inclined at 60° to the beam. A Si(Li) detector positioned at 90° to the beam direction measured the x rays produced in the target. The scattered particles were detected by a silicon surface-barrier detector at 30° with respect to the incident beam.

The targets were made by vacuum evaporation and deposition of the elements Au, Pb, Bi, and U on 15-20 $\mu g/cm^2$ carbon backings. Methods were used to assure that the targets were 99.9% pure and nearly contaminant free.[15] M-shell x-ray spectra were measured for a range of thicknesses (~1 to ~300 $\mu g/cm^2$) for each element and for each charge state of the incident ions in order to ascertain the effects of multiple collisions and to insure that the data presented are for approximately single-collision conditions. M-shell x-ray yields for the thinnest target for each element at the various charge states were normalized to the Rutherford scattered particle yields to determine microscopic M-shell x-ray production cross sections under essentially single-collision conditions.

The efficiency of the Si(Li) detector was determined[16,17] by (1) measuring the X rays emitted from calibrated sources of ^{51}Cr, ^{55}Fe, ^{57}Co, ^{65}Zn, and ^{241}Am, (2) measuring the K-shell x-ray yields per scattered particle from thin Al and Si targets for an incident F^{4+} beam and using available experimental K-shell x-ray production cross sections for Al(K X-ray at 1.487 keV) and Si(K X ray at 1.74 keV), respectively, and (3) calculating the attenuation of the X-rays in the Mylar film, Be entrance window, Au contact layer, and the Si dead layer and normalizing the theoretical curve determined from this attenuation calculation to a measured efficiency point at a higher x-ray energy.

The experimental results will be discussed in terms of the number of K-shell vacancies in the incident projectile. For $q \leq 6$, the cross sections for the production of M-shell X-rays was independent of the number of L electrons within the accuracy of this experiment. If this cross section is taken to be the sum of the DI cross section and the EC(M → L,M,...) cross sections, then either the EC(M → L,M,...) cross sections are small, or the thinnest targets were still thick compared to the mean free path for losing and capturing projectile L electrons. ECPSSR calculations indicate that the cross section for EC(M → L,M,...) is of the order of 1/2% to 1% of the direct ionization cross section for each L vacancy on the projectile. The data and theoretical calculations are shown in Fig. 4.14. The calculations are for the case $q = 6$. Since M_4- and M_5-subshell ionizations dominate the total M-shell ionization, a ratio of the velocity of the incident ion v_1 and the velocity of the target electron in the $M_{4,5}$ subshell, $v_{2M_{4,5}}$, is a good indicator of the velocity ratio regime for our collision systems. The ratio $v_1/v_{2M_{4,5}} = (E_1 n^2/\lambda Z_{2M}^2 R)^{1/2}$ and is ~0.3 to 0.5. Here, E_1 is the projectile energy (laboratory), λ is the ratio of the projectile mass to the electron mass, $n = 3$ is the principle quantum number, $R = 13.6$ eV is the Rydberg constant and $Z_{2M} = Z_2 - 21.15$ for the M_4,M_5 subshells, with Z_2 being the target atomic number. Inferred cross sections for x-ray production due to M-K electron capture may be calculated by substracting σ_{XM}DI + EC(M → L,M,...), shown in Fig. 4.14, from the M-shell x-ray production cross sections for incident fluorine ions with one and two K-shell vacancies. $\sigma_{MX}^{EC(M \to K)}$ is the contribution to the M-shell x-ray production cross section due to EC from the M shell of the target to the K shell of the projectile for two K vacancies present in the bare fluorine ion. $\sigma_{MX}^{EC[M \to (1/2)K]}$ is the contribution to the M-shell x-ray production cross section due to the EC from the M shell of the target to the K shell of the projectile for one K vacancy in the $q = 8$ fluorine. These derived cross sections are shown in Figs. 4.15 and 4.15 together with the comparisons of the data to theoretical predictions of the first Born approximation and

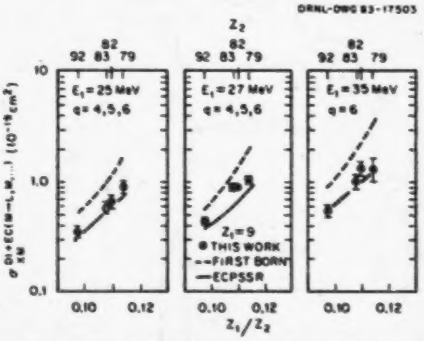

Fig. 4.14. Target M-shell x-ray production cross sections $\sigma_{MX}^{DI+EC(M \to L,M,...)}$ due to DI and EC to L,M,... shells of the projectile versus Z_1/Z_2 for 25-, 27-, and 35-MeV fluorine ($Z_1 = 9$ and $q \leq 6$) with no K-shell vacancies.

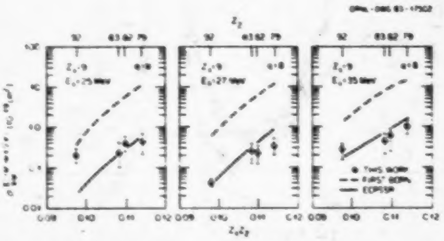

Fig. 4.15. Inferred target (Z_2) M shell to projectile K-shell x-ray production cross section due to EC, $\sigma_{MX}^{EC[M \to (1/2)K]}$ for one K-shell vacancy ($q = 8$) vs Z_1/Z_2.

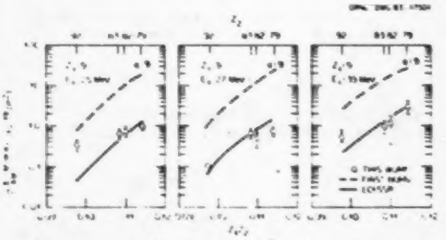

Fig. 4.16. Inferred target (Z_2) M-shell to projectile K-shell x-ray production cross sections due to EC, $\sigma_{MX}^{EC(M \to K)}$ for two K-shell vacancies ($q = 9$), vs Z_1/Z_2.

ECPSSR. In both of these figures, the first Born approximation calculations are displayed by a dashed curve, while the ECPSSR calculations are represented by a solid curve. The theoretical ionization cross sections were converted to x-ray production cross sections for this comparison, with the use of fluorescence yields and Coster-Kronig rates from McGuire.[18]

In both figures, the OBKN EC calculations overpredict the data. Good agreement is evident between predictions of the ECPSSR theory and the data, except for the $_{92}$U data at 25 MeV. An underestimation by the theory of a factor of ~5 is noted at this energy for both q = 8 and 9. The ECPSSR overpredicts the $_{79}$Au and $_{82}$Pb data points at 27 MeV to a lesser degree.

In conclusion, the ECPSSR theory provides a much better estimate of the M-shell x-ray production cross section than the first Born approximation theory. The EC is small for fluorine ions with no K-shell vacancies. The EC contribution to the total M-shell x-ray production cross section is enhanced when the fluorine ions contain vacancies in the K shell. This enhancement, within experimental uncertainties, is twice as large when, instead of one K-shell vacancy, two K-shell vacancies are available on the projectile.

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1. Summary of paper: Physical Review A (in press).
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7. D. E. Johnson, G. Basbas, and F. D. McDaniel, At. Data Nucl. Data Tables 24, 1 (1979).
8. V. S. Nikolaev, Zh. Eksp. Teor. Fiz. 51, 1263 (1966) [Sov. Phys.—JETP 24, 847 (1967)].
9. W. Brandt and G. Lapicki, Phys. Rev. A 23, 1717 (1981).
10. G. Basbas, W. Brandt, and R. H. Ritchie, Phys. Rev. A 7, 1971 (1973).
11. G. Lapicki, Bull. Am. Phys. Soc. 26, 1310 (1981).
12. F. D. McDaniel, J. L. Duggan, G. Basbas, P. D. Miller, and G. Lapicki, Phys. Rev. A 16, 1375 (1977).
13. F. D. McDaniel, A. Toten, R. S. Peterson, J. L. Duggan, S. R. Wilson, J. D. Gressett, P. D. Miller, and G. Lapicki, Phys. Rev. A 19, 1517 (1979).
14. G. Lapacki and F. D. McDaniel, Phys. Rev. A 22, 1896 (1980).
15. P. M. Kocur, J. L. Duggan, R. Mehta, J. Robins, and F. D. McDaniel, IEEE Trans. Nucl. Sci. NS-30, 1580 (1983).
16. R. Mehta, J. L. Duggan, J. L. Price, F. D. McDaniel, and G. Lapicki, Phys. Rev. A 26, 1883 (1982).
17. W. N. Lennard and D. Phillips, Nucl. Instrum. and Methods 166, 521 (1979).
18. E. J. McGuire, Phys. Rev. A 5, 1043 (1972).

COLLISIONS OF MULTIPLY CHARGED NEON IONS WITH WATER VAPOR

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Reaction rate constants of low-energy, multiply charged neon ions with water vapor are measured using a Penning ion trap on-line with the Oak Ridge National Laboratory EN tandem Van de Graaff accelerator. Recoil neon ions are produced inside the ion trap by impact ionization of neon atoms using a pulsed 35 MeV Cl ion beam, foil-stripped to a mean charge state near 10e. The ionization state of stored neon ions is determined by cyclotron resonance in the confining electromagnetic fields. The number of stored ions is detected by resonant axial excitation.[5] Ion loss is mainly due to electron capture from the background gas. Storage times of the order of 100 ms are observed, for neon ions of different charge states, at neon gas pressure up to 10^{-7} Torr. Addition of water vapor into the target chamber is controlled by a separate gas handling system. About 1 cubic centimeter of water is kept in a stainless steel tube and outgassed to remove the dissolved air. Water vapor is admitted into the target chamber via a micrometer adjusted leak valve. Partial pressures of neon gas and water vapor inside the target chamber are determined by using a quadrupole residual gas analyzer and a calibrated ionization gauge. Values of reaction rate constants of multiply charged neon ions with water vapor are obtained from variation of the storage time constants at fixed neon pressure as a function of the water vapor pressure.

Typically, a constant neon partial pressure of 10^{-7} Torr is used while the water vapor pressure is varied from 10^{-8} to 10^{-7} Torr. Previously determined rate constants[6] for Ne^{q+} on neon are used to separate the contributions to the overall rate constant from respective charge exchange collisions of Ne^{q+} with neon and water vapor. Preliminary values of the rate constants indicate they are larger by about one order of magnitude than the corresponding rate constants for Ne^{q+} on Ne collisions.

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5. R. Holmes et al., Bull. Am. Phys. Soc. 27, 513 (1982).
6. D. A. Church et al., Physica Scripta T3, 71 (1983).

ION-ION COLLISION STUDY USING FOLDED BEAM APPARATUS

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A novel apparatus with which charge-changing collisions between identical ions at collision energies relevant to heavy-ion beam transport and storage technology can be investigated was designed, constructed, and thoroughly tested. Essential features of the device are illustrated in Fig. 4.17. A multicharged heavy-ion beam from the ORNL-PIG ion source is bent through a magnetic field, reflected from an electrostatic mirror, folded into the incoming beam, and re-enters the magnetic field where the charge state is analyzed by the same magnet. Charge-changing collisions occur in the collision region where the reflected beam passes through the incoming beam. The oscilloscope trace of intensity profiles (in two orthogonal directions) of a 30-keV Ar^{3+} beam measured with a rotating-wire beam scanner placed at the image plane in the collision region is shown in Fig. 4.18. The upper trace shows the profiles with the reflector turned off and the lower with the reflector on. The positions, shapes, and the intensity of the reflected beam shown in this figure clearly indicate that the device functions in complete accordance with the design objectives.

Recent experience gained from test runs performed using nitrogen and xenon beams indicates that the device can handle all ion species with $q \leq 8$ at collision energies up to 60 kV/q, but it is especially suitable to ions with $A \geq 100$.

The measurement of charge-stripping ($q \rightarrow q + 1$) cross sections for the $Xe^{q+} + Xe^{q+}$ system at 10 kV/q is currently in progress. Because charge-changing ion-ion collisions within beam transport and storage devices can adversely affect the storage lifetimes, the beam intensity and the beam quality, and because a Xe^{q+} beam is a popular heavy-ion driver candidate, the above cross sections are of particular interest to the technology of heavy-ion-beam driven fusion.

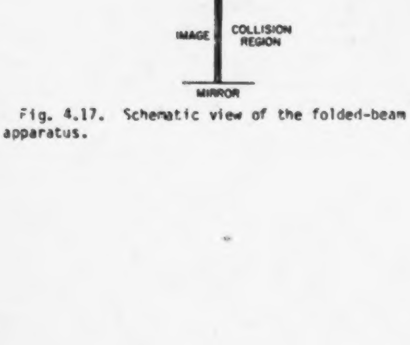

Fig. 4.17. Schematic view of the folded-beam apparatus.

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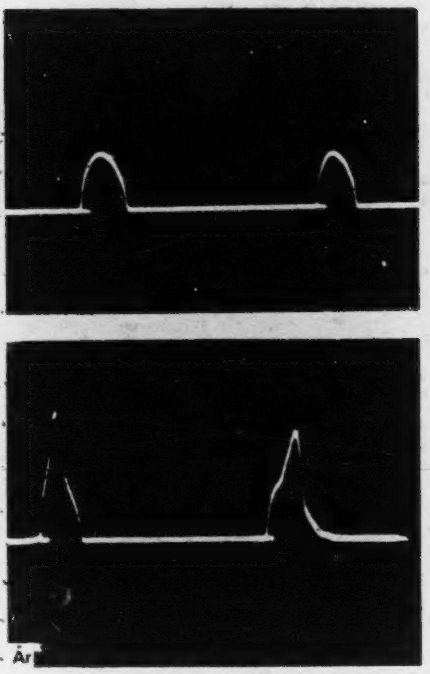

Fig. 4.18. Profiles of Ar^{3+} beam as measured with a scanning wire monitor.

THE EFFECT OF TRANSVERSE CORRELATIONS IN ION CHANNELING IN VERY THIN CRYSTALS[1]

N. Nešković[2]

Theoretical investigations of the problem of ion channeling in crystals have been developed along two major lines. The first one, based on the analytical approach of Lindhard,[3] uses the methods of statistical mechanics, and includes the continuum approximation and the assumption of statistical equilibrium in the transverse plane. The last assumption makes the approach valid only for thick crystals. Within that treatment the effect of correlations between the atomic strings of the crystal is not taken into account. The second line of investigation is based on the Monte Carlo approach in which trajectories of the ions through the crystal are followed.[4] We would also like to mention the calculations of Golovchenko[5] and Ellison et al.[6] Their approaches are with the methods of statistical mechanics, but without the assumption of statistical equilibrium in the transverse plane. Thus, they can be used for thin crystals. The former treatment is analytical and ignores the effect of transverse correlations (TC), while the latter is in general numerical and includes the effect of TC.

The treatment of ion channeling to be presented in this article is valid only for very thin crystals. It uses the methods of ion-molecule scattering theory, to analyze the probability of transmission of the ions as a function of impact parameter, and the Monte Carlo method, to obtain the angular distribution of transmitted ions. The approach is based on the momentum approximation within which the effect of longitudinal correlations (LC) is neglected. However, it enables a proper treatment of the effect of TC. When compared to the trajectory following Monte Carlo calculations, this calculation is less accurate, but its simplicity enables one to work with a much greater number of ions and thus achieve a substantially higher angular resolution.

Let us take the z axis to coincide with the channel axis and the origin to lie in the median plane of the crystal. The incident ion velocity is parallel to the z axis. The crystal is assumed to be sufficiently thin for the ion trajectory to be approximated by a straight line. In this case one can apply the momentum approximation. Within this approximation the x and y components of the scattering angle, $\vec{\theta}$, are

$$\theta_x = -\frac{1}{2E}\sum_{i=1}^{M}\sum_{k=1}^{N}\int_{-\infty}^{\infty}\partial_x U_{ik}dz$$

and

$$\theta_y = -\frac{1}{2E}\sum_{i=1}^{M}\sum_{k=1}^{N}\int_{-\infty}^{\infty}\partial_y U_{ik}dz, \qquad (1)$$

where E is the incident energy, $U_{ik} = U_{ik}(x,y,z)$ the interaction potential of the ion and the kth atom of the ith atomic string of the crystal, M the number of atomic strings, and N the number of atoms in one string (it is assumed, for the sake of simplicity, that all the strings have the same number of atoms); $\partial_x \equiv \partial/\partial_x$ and $\partial_y \equiv \partial/\partial_y$. These expressions show that, from the point of view of components of $\vec{\theta}$, the (MN+1)-particle collision under consideration reduces to MN independent 2-particle collisions, i.e. the effect of multiple scattering (MS) cannot be observed.[7] It is clear that contributions of the atoms of one string to the components of $\vec{\theta}$ do not depend on their positions within the string. Thus,

$$\theta_x = -\frac{N}{2E}\sum_{i=1}^{M}\partial_x V_i$$

and

$$\theta_y = -\frac{N}{2E}\sum_{i=1}^{M}\partial_y V_i, \qquad (2)$$

where V_i is the integral of the interaction potential of the ion and one of the atoms of the ith atomic string. These expressions show that the process we analyze in fact consists (from the point of view of components of $\vec{\theta}$) of M independent 2-particle collisions. Thus, applying the momentum approximation we neglect the fact that the atoms of one string are arranged in a non-random way, i.e. the effect of LC.

In the case under consideration the differential scattering cross section is $\sigma = |J|^{-1}$ where $J = \partial_x\theta_x\partial_y\theta_y - \partial_y\theta_x\partial_x\theta_y$.[8,9] The variable J can be expressed as $J = J_0 + J'$,[7] where

$$J_0 = \sum_{i=1}^{M} J_{ii}, \quad J' = \sum_{i=1}^{M}\sum_{j=i+1}^{M}(J_{ij} + J_{ji}) \qquad (3)$$

and

$$J_{ij} = \left(\frac{N}{2E}\right)^2 (\partial_{xx}V_i\partial_{yy}V_j - \partial_{xy}V_i\partial_{xy}V_j). \qquad (4)$$

Term J_{ii} describes the scattering from the ith atomic string of the crystal, and the sum of terms J_{ij} and J_{ji} describes the coupling between the ith and jth atomic string as seen by the ion. Hence, from the point of view of σ the (MN+1)-particle collision in question does not reduce to MN independent 2-particle collisions, i.e. the effect of MS can be observed.[7] In this case the process we analyze consists of M non-independent 2-particle collisions. We want to emphasize that this is an interference effect: contributions of the atomic strings to σ interfere.

It is obvious that equation $J' = 0$ defines the line along which the effect of MS is not observable.[7] We may call this line the single scattering line (SSL). The rainbow line (RL), i.e. the line along which σ is infinite,[8,9] is given by equation $J = 0$. These lines are defined either in the impact parameter plane (the transverse plane) or in the scattering angle plane.

Let us now concentrate on the transmission of H^+ ions through the <110> channel of a Si crystal. The incident energy will be 7 MeV, and the crystal will be ≈1500 Å thick (N = 392). We shall assume that the ion-atom interaction potential is of the Thomas-Fermi type, and for the integral of that potential along the z axis we shall use Lindhard's expression $V_i = Z_1Z_2e^2 \ln(Ca^2/\rho_i^2 + 1)$,[3] where $Z_1 = 1$ and $Z_2 = 14$ are the atomic numbers of the projectile and the target, respectively, e is the unit charge, a is the screening length, $\rho_i^2 = (x-x_i)^2 + (y-y_i)^2$, x_i and y_i are the coordinates of the ith atomic string of the crystal, and C = 3 is a fitting parameter.

Fig. 4.19 shows the SSL and the RL in the impact parameter plane in this H^+ + Si case. The number of atomic strings of the crystal is 20, i.e. we took into account the strings lying on the four nearest (relative to the channel axis) coordination circles. It is clear that the SSL connects the regions in the impact parameter plane in which the scattering process under consideration is dominated by the interaction with one atomic string. On the other hand, the

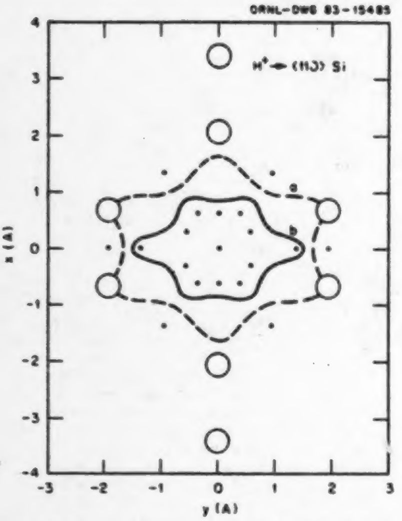

Fig. 4.19. The SSL (a), the RL (b) and the stationary points of σ in the impact parameter plane.

RL lies in the region of the impact parameter plane where the contributions of more strings are important. It must be emphasized that the lines given in Fig. 4.19 are determined only by the arrangement of the atomic strings and the screening length. This figure also shows the stationary points of σ in the impact parameter plane. At the origin this variable is maximal and at the other eighteen points it is minimal. The SSL and the RL were also analyzed in the cases of 6, 8 and 12 atomic strings, i.e. one, two and three coordination circles, respectively. The result is that the strings lying on the second did and those lying on the third and fourth coordination circles do not influence the shape of those lines.

Fig. 4.20 gives the dependence of σ on parameter $\rho = (x^2+y^2)^{1/2}$ for $\phi = \tan^{-1}(y/x) = 30$ and 210°; the number of atomic strings of the crystal is 20. This figure also contains the differential scattering cross section when term J' is not taken into account, i.e. when the effect of MS is neglected. These two curves clearly demonstrate that the rainbow effect is a consequence of MS, i.e. of the fact that contributions of the atomic strings to the probability of transmission of the ions interfere.

The RL in the scattering angle plane is shown in Fig. 4.21. The circles appearing in this figure represent the last atoms of the atomic strings of the crystal lying on the first two coordination circles; the angles corresponding to these circles are determined by the z axis and the lines defined by the origin and these

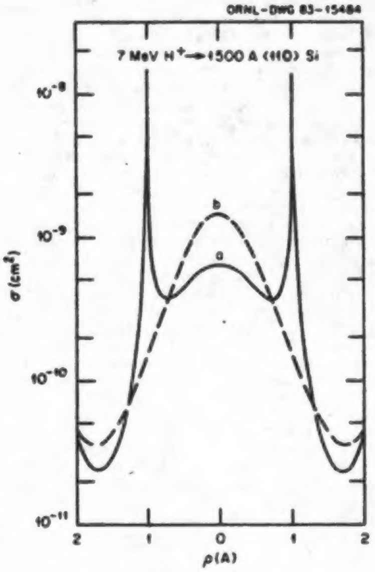

Fig. 4.20. The dependence of σ on ρ for ϕ = 30 and 210° with (a) and without (b) the effect of MS.

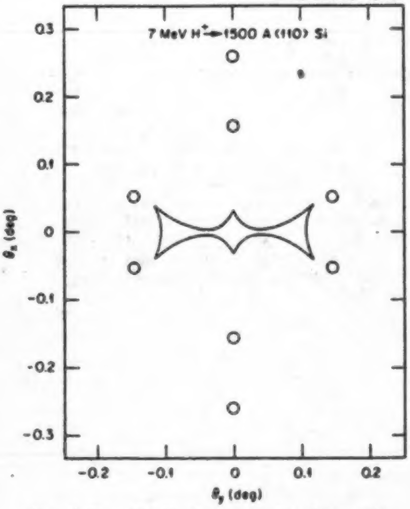

Fig. 4.21. The RL in the scattering angle plane.

atoms. It is important to note that the approximation used (within which the effect of LC is neglected) does not give correct results in the vicinity of these circles. This is related to the extreme left and right parts of the RL shown in this figure. Let us, therefore, concentrate on the central part of the RL, i.e. on the region in which the scattering angle is less than ~ 0.04°. In this region the RL looks as if it has four points, each of them directed towards a pair of atomic strings of the crystal. When the focusing corresponding to the channel center is taken into account one can expect in this region a complex distribution of transmitted ions. For lower incident energies and/or thicker crystals the dimensions of the RL are larger (see Eqs. 2). It must be noted that, although the approximation we use is more accurate for higher energies and/or thinner crystals, values of 7 MeV and ≈1500 Å were chosen taking into account the difficulties in making very thin crystals and detectors with high spatial resolution.

We also analyzed the influence of the effect of thermal vibrations of the atomic strings of the crystal. The calculation showed that changes of the coordinates of the SSL and the RL due to this effect were very small.

The angular distribution of the transmitted ions is given by $\sigma = f[x(\theta_x,\theta_y), y(\theta_x,\theta_y)] = g(\theta_x,\theta_y)$. However, variables x and y are very complicated multivalued functions of θ_x and θ_y.[9] Therefore, in order to avoid mathematical difficulties, the Monte Carlo method was used. Values of parameters x and y were chosen randomly within the (hexagonal) region of the channel, and, according to the calculated values of θ_x and θ_y, each particle was recorded as if it had entered a bin in the scattering angle plane. The calculation was performed with Eqs. (2) with the effect of thermal vibrations included; the number of atomic strings was 8, while the number of ions was ≈ 1.3 × 10^6. Fig. 4.22 gives the yield of the transmitted ions as a function of θ_x for θ_y between 0 and 0.002° (see Fig. 4.21). It was found that in this case, for the rainbow effect to be observed, an angular resolution higher than ~ 0.004° was needed.

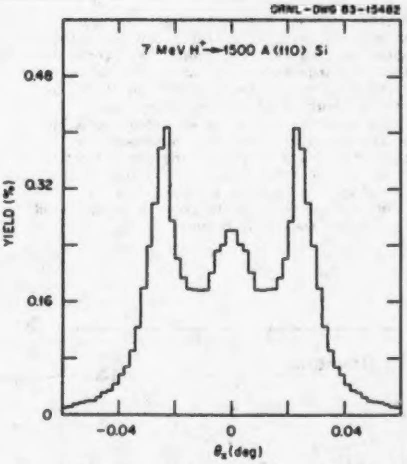

Fig. 4.22. The yield of the transmitted ions as a function of θ_x and θ_y between 0 and 0.002°.

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1. Summary of paper submitted for publication in Physical Review Letters.

2. Boris Kidrič Institute of Nuclear Sciences, Belgrade, Yugoslavia.

3. J. Lindhard, Mat. Fys. Medd. Dan. Vid. Selsk. 34, No. 14 (1965).

4. See, e.g., J. H. Barrett, Phys. Rev. B 3, 1527 (1971).

5. J. A. Golovchenko, Phys. Rev. B 13, 4672 (1976).

6. J. A. Ellison, S. T. Chui and W. M. Gibson, Phys. Rev. B 18, 5963 (1978).

7. N. Nešković, B. Perović and D. Ćirić, Phys. Lett. 96A, 183 (1983).

8. I. V. Komarov and A. P. Shcherbakov, Vestnik LGU 16, 24 (1979), in Russian.

9. Yu. N. Demkov, Sov. Phys.-JETP 53, 63 (1981).

RADIATION FROM CHANNELING OF RELATIVISTIC ELECTRONS AND POSITRONS

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Energetic electrons entering a crystal in low index planar directions can be trapped into bound states of the potential made up by the atoms in the planar sheet. This potential has associated eigenstates analogous to an averaged one dimensional atom. Similarly electrons injected in an axial direction are bound into eigenstates of the two dimensional "string" potential characterized by two quantum number n,ℓ. When positrons are injected in planar directions they are bound between the atomic sheets into an almost harmonic potential. We have observed radiation arising from bound state transitions in all the above configurations[3] in a number of materials e.g., C,[4,5] Si,[6-8] Ge,[9] W, LiF,[10,11] LiH, BeO.

The work reported here is the result of a collaborative program, between ORNL, LLNL, and the Department of Electrical Engineering at Stanford University, which has been underway for about four years. Our group was the first to report experimental observation of both positron and electron channeling radiation and has produced numerous publications in this subject area. For all of this work the LLNL electron-positron LINAC was used for producing beams of 17-54 MeV electrons and 54-82 MeV positrons.

In this brief report we concentrate on a comparison of electron and positron planar channeling radiation spectra with theory for simple crystals and the effect of "platelet" defects in diamond on these spectra. Planar channeled electrons are bound into eigenstates of a single one dimensional sheet potential. These states are characterized by a single quantum number, n and dipole selection rules dictate Δn odd. The spectrum can be calculated from a solution of the one dimensional Schrödinger equation using the many-beam formulation for the transverse motion. A comparison tween theoretical and measured line positions and intensities for 54.4 MeV electrons in the three principal planes in diamond is shown in Fig. 4.23.[4] The agreement is quite good as exemplified in Table 4.5 for the (110) plane.

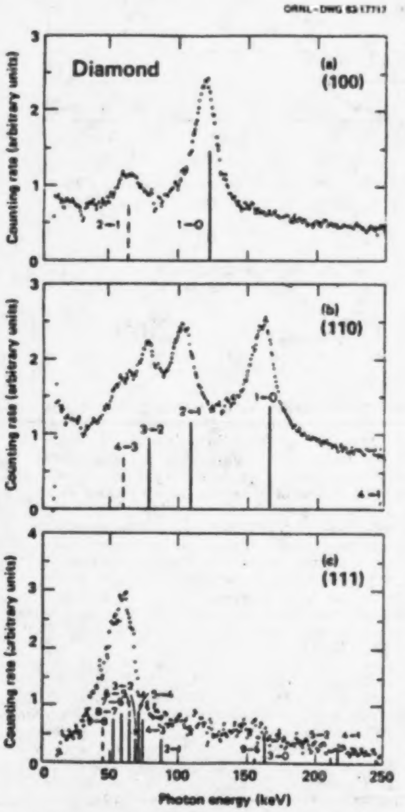

Fig. 4.23. Radiation spectra for 54.5 MeV electrons channeled along the (a) (100), (b) (110) and (c) (111) planes in diamond (23 μm thick). The positions of the vertical lines indicate the calculated positions and relative intensities for Δn = 1 transitions.

Table 4.5. Characteristics of channeling radiation for 54.5 MeV ($\gamma = 107.6$) electrons along the (110) plane in diamond (in keV).

Transition	E_{calc}	E_{exp}
1 → 0	164.8 ± 0.07	165.0
2 → 1	106.9 ± 0.06	105.2
3 → 2	80.0 ± 0.04	79.4
4 → 3	≈59.2	≈60

Positrons are repelled from the positive cores making up the single plane and are bound in the potential formed from two adjacent planes. This two plane potential is almost harmonic and all lines appear in the same energy region. Since the atomic potentials involved are the same as those used in calculating the electron spectra the positron spectrum should be equally well described. However, as seen in Fig. 4.24 for 54.4 MeV positrons in (111) diamond, the predicted spectrum is too high in energy by ~5%. (These same effects are observed in e^- and e^+ channeling radiation in Si.) The causes for these discrepancies, which are also observed in the other planar directions, is not yet understood.

Effects of "Platelet" Defects on Electron and Positron Channeling Radiation

As can he seen from the above, the study of channeling radiation is at a stage of development where small differences between theory and experiment in well ordered crystals become interesting and where the effects of crystal imperfections on channeling radiation spectra might be used as a diagnostic tool to characterize crystal defects. A start in this direction has been made in a study of the effect of platelet defects in diamond on channeling radiation from 54 MeV positrons and electrons. In naturally occurring diamonds, one type which occurs (classified Type-Ia) contains

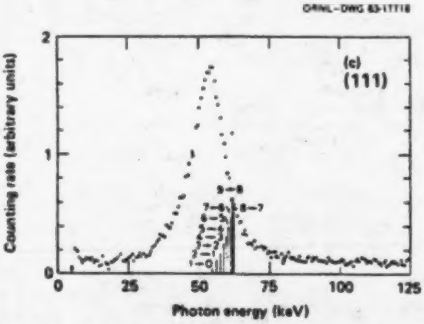

Fig. 4.24. Radiation spectrum for 54.4 MeV positrons channeled along the (111) direction in diamond.

nitrogen impurities in the form of aggregates which are responsible for an absorption peak at 7.8 μm. Some Type-Ia diamonds have an absorption peak at 7.3 μm resulting from the presence of platelets. These are thought to be single layers of atomic nitrogen inserted between (100) planes. When viewed along this direction the defect would have an appearance similar to a dislocation but when viewed along the (110) or (111) planar directions the defect would appear as a stacking fault. Hence one might expect anisotropic differences in the effect of these defects on channeling radiation from diamond. Strong effects have indeed been found which depend not only on crystalographic direction but also upon whether electrons or positrons are used as a probe. An example is given in Fig. 4.25 which shows positron and electron spectra taken in the (110) direction of platelet-free (Type-IIa) and platelet containing (Type-Ia) diamond. Comparing the positron spectra (Figs. 4.25a and 4.25c) one finds a reduction in intensity of a factor of ~5; the remaining peak is at the same position but it is reduced in width by almost a factor of 2! Comparing the electron spectra (Figs. 4.25b and 4.25c) one finds that the defects cause a complete obliteration of channeling radiation structure. This in contrast to the e.g. (111) spectrum (not shown) which is almost unaffected by the presence of platelets. A qualitative explanation for these effects can be made in terms of preferential de-channeling but regardless of whether or not these phenomena are currently understood in detail, it does appear that channeling radiation might have a use in delineating types and concentrations of impurities or defects in crystals.

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1. Lawrence Livermore National Laboratory.
2. Department of Electrical Engineering, Stanford University.

3. S. Datz, Proc. Conf. on X-ray and Inner-Shell Physics, AIP Conf. Proc. No. 94, ed. B. Crasemann (1982), pp. 723-735.
4. S. Datz et al., Phys. Lett. 96A, 314 (1983).
5. S. Datz et al., Nucl. Instrum. Meth., in press.
6. M. J. Alguard et al., Phys. Rev. Lett. 42, 1148 (1979).
7. R. L. Swent et al., Phys. Rev. Lett. 43, 1723 (1979).
8. R. L. Swent et al., Nucl. Instrum. Meth. 194, 235 (1982).
9. H. Park et al., Phys. Lett. 96A, 45 (1983).
10. B. Berman et al., Phys. Rev. Lett. 49, 474 (1982).
11. R. L. Swent et al., Phys. Rev. B, 1983, in press.

TWO-DIMENSIONAL "MOLECULAR" BOUND STATES FOR CHANNELED ELECTRONS

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Axially channeled electrons are captured into bound states of the row or "atomic string" potential. When two rows lie in close proximity as in the case of the <110> direction in diamond the potential overlaps, forming a saddle point between the rows. The potential for 4 MeV electrons in <110> diamond is shown in the upper portion of Fig. 4.26. Solving for the eigenstates of this potential one finds that the 1s states are well localized to a single row. However, the 2p lies above the saddle point and splits into four molecular type levels. The resultant

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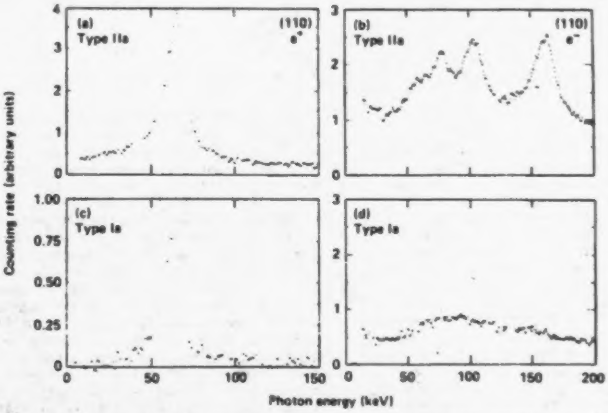

Fig. 4.25. Comparison of 54.5 MeV electron and positron channeling spectra in (110) diamond for type-IIa (platelet-free) and type-Ia (platelet-containing) specimens.

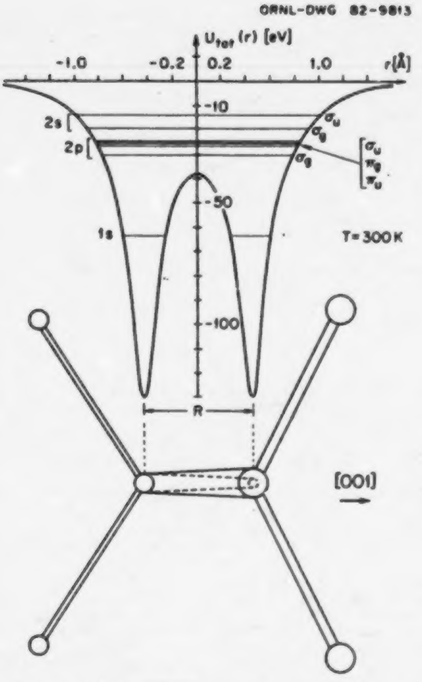

Fig. 4.26. (Upper) Potential and energy levels for 4 MeV electrons channeled along <110> axis in diamond. (Lower) Atomic core and bond configuration in diamond viewed along the <110> direction.

spectrum shown in Fig. 4.27 gives evidence for this effect.[2]

The qualitative features are obtained in a simple treatment analogous to the linear-combination-of-atomic-orbitals (LCAO) method in chemistry. When the transverse Hamiltonian is diagonalized in the subspace spanned by the four single-string 2p states for a pair of strings, four eigenstates are obtained which may be classified according to their symmetry under reflection in the midpoint between the strings, gerade and ungerade, and under reflection in the line connecting the two strings, σ and π. The line energies for transitions between molecular energy levels obtained from the LCAO treatment are given in Table 4.6 together with the single-string values obtained from a solution to the two-dimensional Schrödinger equation. Mixing with the near-lying 2s levels turns out to be quite strong. In particular, the $\sigma_u 2p$ level is lowered considerably when mixing with the $\sigma_g 2s$ state is introduced. The splitting between the lines is seen to increase by ~ 150 eV so that it is now ~ 100 eV

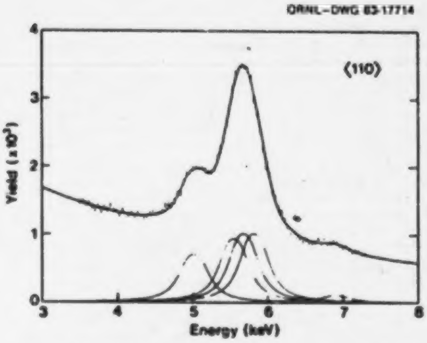

Fig. 4.27. Decomposition of the <110> 2p-1s and 2s-1s lines (see Table 4).

larger than the observed splitting. Also, a dipole transition 2s-1s becomes allowed, and a corresponding weak line is visible in the spectrum (see Fig. 4.27). While the LCAO-type model is very instructive for qualitative purposes, its accuracy is limited and difficult to assess.

Table 4.6. Photon energies (in eV) for 2s-1s and 2p-1s transitions for 4-MeV electrons in <110> diamond.

Transition	Single string	First order LCAO	With 2s-2p mixing	Many Beam	Experiment
$\sigma_g 2s-\sigma_u 1s$			7253	7103	6933
2p-1s	5810				
$\sigma_u-\sigma_g$		6025	6015	6019	5897
$\pi_g-\sigma_u$		5888		5887	5751
$\pi_u-\sigma_g$		5771		5742	5624
$\sigma_g-\sigma_u$		5279		5090	5084

The values obtained for channeling radiation energies from the many-beam formulation are listed in Table 4.6. For the 2p-1s transitions, there is reasonable agreement with the result of the LCAO-type calculations. The upper three lines and the 1s-2s line are higher than the measured values by ~ 120 eV. However, the most significant deviation is for the separation of the σ_g–σ_u line which is larger by ~ 130 eV than deduced from the experiment. This has been attributed to the accumulation of charge in the tetrahedral bonds in diamond. The reason for this charge accumulation can be seen in the lower portion of Fig. 4.26. Each atom in a <110> row is bonded to two atoms in a neighboring row and to one atom in each of the next-nearest neighboring row. Hence, accumulation of charge in the bonds increases the electron density between close-lying pairs of <110> rows and increases the potential energy of channeled electrons in this region. Since the $\sigma_g 2p$ state has a high density here, this level will increase in energy relative to that of other 2p levels, i.e., the splitting will be reduced, as required by experiment. With the use of the many-beam method and the Gaussian parameters obtained from the x-ray analysis, the energy levels have been recalculated as a function of the electron density enhancement and the closest match with the observed splitting is obtained for an electron density of $1.7/\text{Å}^3$ in the center of bonds. Although this determination is probably less accurate than that obtained from the x-ray data, it does demonstrate that information on charge distributions and potentials in crystals can be obtained from channeling radiation.

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1. Physics Institute, University of Aarhus, Aarhus, Denmark.
2. J. U. Andersen et al., Rev. Lett. 49, 215 (1982)

EN TANDEM OPERATIONS

G. F. Wells P. D. Miller
P. L. Pepmiller

During the past year the EN tandem has logged slightly less than 2,000 hours in support of experimental research efforts. The conversion from a nuclear physics facility to a high energy atomic physics facility is now complete, as it has been over a year since any nuclear physics experiments have been performed using the EN.

During the summer of 1983 machine reliability at high voltages degraded substantially. Due to column insulator and tube damage it became necessary to reduce the resistance or short out over thirty planes in the high energy column. It was decided to do a rather complete overhaul of the accelerator. This included thorough cleaning, rebuilt tubes, reworked resistor holders, and a new belt. This work is going on at the time of this writing.

Upgrading of the vacuum system is still progressing with the purchase and installation of cryopumps and other high vacuum apparatus. Almost all beam lines between the 90° magnet, and the end of either switching magnet have now been improved as have approximately half of the experimental beam lines. The next planned upgrade involves the region between the sources and the generator. The installation of the Elbek magnetic spectrometer is essentially completed, lacking only some details. An Alton-Aarhus-type ion source has been purchased and is being tested.

8.3 High Flux Isotope Reactor (HFIR)

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

Answer: NEUTRON SCATTERING

(a) The new science being explored by the neutron scattering program at HFIR includes the studies of:

1. The long-range orientational alignment of atomic nuclei at ultralow temperatures (10^{-3} K)
2. The new state of condensed matter arising from the coexistence of magnetism and superconductivity
3. The relationship of long-range magnetic correlations, spatial dimensionality and random magnetic fields
4. The relationship between periodic lattice distortions and superconductivity in uranium compounds
5. The interatomic forces in materials (the A15 compounds) having the highest known superconducting transition temperatures
6. The interactions between magnetic atoms in magnetic-glasses and amorphous materials
7. The interactions between atomic vibrations and the electronic transitions responsible for valence fluctuations in compounds containing cerium, samarium or thulium
8. The quantized flux lines in superconductors
9. The microscopic motion of water inside biological cells
10. The new materials obtained by inserting atomic layers of various elements or compounds between atomic layers of carbon in graphite.

(b) The neutron scattering facilities at the HFIR are designed to exploit the highest neutron flux in the world. They are used to obtain very important fundamental microscopic information on materials that is impossible or very difficult to obtain by other experimental techniques. By direct probing of the static and dynamic structure of materials, neutron scattering experiments provide information that is necessary for understanding the results of many other types of research and vital in the prediction and development of new materials that have special physical properties. In the research at HFIR particular emphasis is placed on investigations that will help to develop materials required for advanced energy technologies. The principal types of research techniques include neutron diffraction, inelastic neutron scattering, and polarization analysis. Neutron diffraction measurements are performed to investigate crystalline and magnetic structures and phase transitions. Inelastic neutron scattering experiments determine lattice vibrational and magnetic excitation energies and line widths, which give direct information on the electrical and magnetic forces existing between atoms in materials. Polarized-beam diffraction and polarization-analysis techniques are used to determine the magnetic density within atoms and the magnetic moment distribution in alloy systems. Sample environment facilities are exploited to investigate materials properties at temperature extremes (5×10^{-4} K to 2×10^3 K), at high pressures (30,000 atm) and at high magnetic fields (60,000 gauss). New high-sensitivity-neutron detectors and high-speed data acquisition systems are being exploited for studies of the kinetics of transient phenomena such as phase changes. These various types of techniques and facilities are utilized to provide important results in all areas of materials science, because the intimate relationship between physical properties and structural properties is at the very core of understanding materials. Recent neutron scattering investigations at HFIR have involved studies in the fields of magnetism, superconductivity, lattice dynamics, hydrogen diffusion, biology, defects, disordered materials, liquids, amorphous materials, and polymer configurations.

MATERIALS FOR FUSION REACTORS

The 14.1-MeV neutrons in a fusion power reactor generate large quantities of helium and hydrogen in the lattice of the blanket structural material. These gases alter the normal neutron irradiation response in ways that are not yet understood. Fusion materials containing nickel are being irradiated in HFIR to simulate the fusion environment. Fast neutrons create displacement damage and helium and hydrogen are produced by (n,p) and (n,α) reactions, the latter primarily from nickel. These studies will lead to a fundamental understanding of the effects of 14-MeV neutrons and to a data base for design with austenitic and ferritic stainless steels.

TRANSPLUTONIUM RESEARCH

The science being addressed worldwide in transplutonium research with HFIR-produced elements is detailed in the National Academy of Science publication, "Opportunities and Challenges in Research with Transplutonium Elements,'' 1983.

2. What are this facility's unique features (i.e., not duplicated elsewhere?

NEUTRON SCATTERING

The unique features of the neutron scattering facilities at the HFIR exist primarily because of the very high thermal neutron source flux provided by the reactor. At the reactor end of the beam tubes, the thermal neutron flux is about 1.5×10^{15} n/cm^2/sec, which is the highest in the United States and matches that at the Institut Laue-Langevin as the two highest in the world.

Unique neutron scattering facilities have also been provided for particular types of research. These include:

(1) Very-high-resolutiondouble-perfect-crystal small-angle scattering spectrometer.

(2) Time-of-flight neutron spectrometer utilizing an electrically-pulsed monochromator system with time focusing. This spectrometer is much more flexible than most time-of-flight spectrometers, and it has the capability of using pseudo-random pulsing and associated cross-correlation techniques to permit an extremely high duty cycle.

(3) Triple-axis polarization analysis spectrometer to permit both energy analysis and polarization analysis of the scattered neutron beam.

IRRADIATIONS

The HFIR has a usable neutron flux for irradiations of approximately 2.5 x 10^{15} n/cm^2/sec in a cylindrical volume of approximately 13 cm dia by 50 cm. This is the highest average flux available in the world. The combination of HFIR irradiations capabilities and the TRU separations and preparation facilities renders HFIR/TRU the unique source for the free world of transplutonium elements.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

Answer: NEUTRON SCATTERING

The types of research instrumentation at the HFIR for neutron scattering experiments are described in the attached brochure. These include:

(1) 2-axis diffractometers for elastic neutron scattering investigations, such as chemical structures, magnetic structures, and the structures of liquids.

(2) 3-axis spectrometers for inelastic neutron scattering investigations, such as phonon and magnon energy levels, atomic and molecular energy levels, and lattice dynamics.

(3) Time-of-flight spectrometer for inelastic neutron scattering investigations of the excitation energy spectra of crystalline and amorphous solids and of the momentum distributions of the atoms in liquids. This spectrometer utilizes an electrically-pulsed monochromator system with time focusing, and it has the capability of using pseudo-random pulsing and associated cross-correlation techniques to permit an extremely high duty cycle.

(4) Polarization-analysis spectrometer for neutron scattering investigations of magnetic density and magnetic excitation energies that require polarization analysis, as well as energy analysis, of the scattered neutron beam.

(5) Very-high-resolution double-perfect-crystal small-angle scattering spectrometer. This spectrometer has provided very valuable data in investigations of flux-line-lattices in Type II Superconductors.

(6) 30-m small-angle scattering camera, which is part of the National Center for Small-Angle Scattering Research (NCSASR). This camera is utilized in studying structures of dimensions from a few tens to a few thousands of angstroms.

(7) One-dimensional and two-dimensional neutron cameras for studying structural changes in real time.

(8) Auxiliary equipment for changing the sample environment:

- (a) Ultralow temperature (10 mK) refrigerators
- (b) High temperature (1700 C) furnaces
- (c) High pressure (30 kbar) devices
- (d) Superconducting magnet (60 kgauss).

IRRADIATIONS

(1) A hydraulic tube facility, which permits samples to be inserted and withdrawn from the reactor during operation, is available for the production and subsequent study of radionuclides.

(2) A high sensitivity neutron activation analysis facility, which utilizes the hydraulic tube, is also available. The irradiated specimens are removed from the reactor into a hot cell for processing and analytical determinations.

(3) The HFIR provides the ability to study the effects of intense gamma radiation on the properties of materials. Gamma-ray flux as high as 8×10^7 R/hr is available in the central core region of spent fuel elements which are stored in the reactor pool.

(4) The sister facility, TRU, for the processing of transuranium elements, is discussed in the ORNL response to these questions for TRU.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1981 and FY 1985?**

Answer: NEUTRON SCATTERING

Research highlights during the period FY 1981 present include the following:

(1) Determination of the coexistence of ferromagnetism and superconductivity in a erbium-rhodium-boron alloy. This definitely showed the coexistence of ferromagnetism, a sinusoidally-modulated magnetic structure, and superconductivity in a small temperature region between 0.72 and 1.2 K, won a DOE award in 1982 as the outstanding scientific accomplishment in solid state physics.

(2) Determination of the momentum distribution in ^{4}He. This research verified the existence of a condensate state in superfluid ^{4}He, which amounts to about 11% at 1 K. The amount of condensate decreases rapidly with small increases in pressure.

(3) Determination of nuclear magnetic order in the mK temperature region. The first observations of nuclear magnetic ordering by neutron diffraction have been made on praseodymium-tin and praseodymium-copper alloys and holmium-vanadium mixed oxide in the mK temperature region. These experiments open up a completely new area of research for studying enhanced nuclear magnetism.

(4) Small-angle scattering of flux-line lattices in Type II Superconductors. The first measurements of a flux-line lattice in the class of high-temperature superconductors with the A15 structure have been made on vanadium-three-silicon. Determination of the temperature-dependent low-field penetration depth X provides insight into the origin of superconductivity in this material.

(5) Determination of the spin structure copper-manganese spin glass. Polarization analysis measurements show both ferromagnetic and antiferromagnetic correlations; the interaction between the ferromagnetic and antiferromagnetic regions is probably responsible for the unusual magnetic behavior of these spin-glass alloys.

(6) Determination that lattice vibrations interact strongly with the electronic transitions responsible for the valence fluctuations in compounds containing cerium, samarium, or thulium.

(7) Determination that the microscopic motion of H_2O molecules in biological cells is not the same as that in ordinary water, but is strongly influenced in a complicated way by the presence of protein material in the cells.

(8) Determination that long-range magnetic ordering can exist in materials containing internal random magnetic fields.

(9) Determination of the interatomic forces and structural phases of the new materials obtained by intercalating graphite with two-dimensional layers of alkali metals.

(10) Determination of the ionic hydration in aqueous solutions. These studies involved measurements on several neodymium trichloride solutions in heavy water (D_2O) having different isotopic states of neodymium or chloride ions. The mechanism by which ions pass through biological membranes depends on hydration.

(11) The structure of liquid water, described by the three distribution functions for oxygen-oxygen, oxygen-hydrogen, and hydrogen-hydrogen interactions, has been uniquely determined for the first time by neutron diffraction from light water (H_2O) and heavy water (D_2O) mixtures.

Research highlights anticipated for the remainder of FY 1984 and FY 1985 include:

(1) Investigations of enhanced nuclear magnetism at temperatures down to 0.5 mK.

(2) Real-time measurements of structural changes in materials using one-dimensional and two-dimensional cameras.

(3) Investigations of the momentum distribution in mixtures of the quantum fluids ^{4}He and ^{3}He.

(4) Investigations of the magnetic excitations in spin-glass materials and random-field magnetic systems.

(5) Investigation of the magnetic and crystalline structures of $EuMo_6S_8$, the only known material to become superconducting under pressure.

FUSION ENERGY PROGRAM

Type 316 stainless steel has been found to have a useful life of 5 MW-year/m^2 in a fusion reactor at temperatures up to 500 C. Improved austenitic stainless steel, the prime-candidate alloy (PCA), has a projected life of at least 10 MW-year/m^2 based on microstructural evolution of HFIR-irradiated samples. Ferritic steels, HT-9 and modified 9 Cr-1 Mo, have been found to be highly swelling resistant, but do show helium bubbles at 4 MW-year/m^2. Tests at higher fluences are underway. The HFIR results have given better understanding of the fusion environment and increase our confidence that fusion reactors will have acceptable lifetimes.

FISSION REACTOR PROGRAM (GAS COOLED REACTOR)

The HFBR provided test facilities for comparison of irradiation performance of four candidate fissile particle types for low-enriched uranium (LEU) HTGR fuel capsules. Tests in numerous capsules provided data used in selection of Triso-coat $UC_{0.4}O_{1.6}$ as a reference fuel particle for HTGR lead plant. Test facilities were also provided for gathering dimensional stability data for candidate side reactor graphites. Under a program of international cooperation with the Federal Republic of Germany, candidate side reflection graphites for the German Pebble Bed High Temperature Reactor were irradiated in the HFIR target capsules.

TRANSPLUTONIUM PRODUCTION PROGRAM

Researchers throughout the free world are dependent on HFIR-TRU for transplutonium elements. Fifty-one transplutonium element targets were irradiated and then transferred to the Transplutonium Processing Plant (TRU) where they were processed to yield berkelium-249, californium-252, einsteinium-253, and fermium-257, the heaviest nuclide which can be produced in a reactor irradiation. A total of 92 shipments of purified products were made to research institutions both in the U.S. and abroad. Special target assemblies containing iron-54, tin-118, and radium-226 were also irradiated in the HFIR target island for production of unusual isotopes.

ACTIVATION ANALYSIS PROGRAM

The determination of uranium and thorium in high purity materials used to manufacture semiconductor memories was investigated by high-fluence neutron activation analysis. The impetus for this study was the so-called "soft error" effect in computer memories caused by the ionizing alpha particles emitted by uranium and thorium and their daughters.

NUCLEAR MEDICINE AND BIOMEDICAL TECHNOLOGY PROGRAM

Osmium-191 produced in high yields in the HFIR is used for first-pass radionuclide angiography for the detection and quantification of intracardiac shunts. It has an extremely low absorbed radiation dose to the patient and repeat studies can be performed. Osmium-192 is also distributed to Medical Cooperative Program participants and used to evaluate generator performance.

ISOTOPES PROGRAM

In addition to ongoing programs to produce iridium-192 and calcium-47, irradiations to produce several thousand curies of greater than 150 Ci/g cobalt-60 were initiated. This grade has wide application in teletherapy machines for the treatment of cancer. A 2-year high flux irradiation of low specific activity targets to produce 1000 Ci/g cobalt-60 was completed. The ultra-high specific activity cobalt-60 was used for precise radiography of thick or dense materials. Gadolinium-153 was produced for use in bone density studies and the diagnosis of osteoporesis.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: NEUTRON SCATTERING

Facility additions are:

(1 A 30-meter Small-Angle Neutron Scattering Facility, part of the National Center for Small-Angle Scattering Research, is used for studies of global structures (10 - 1000 A) in polymers and polymer blends, biological systems, oil shales, voids in irradiated materials, and metal alloys.

(2) A Wide-Angle Neutron Diffractometer, built with Japanese funds as part of the U.S.-Japan Cooperative Program in Neutron Scattering, includes a linear position-sensitive neutron detector and a high-speed data-acquisition system for time-slicing measurements on phase-change kinetics.

(3) Cryogenics Laboratory/User Office Annex to be built in FY 1984 with GPP funds is to be used for setting and testing cryogenics facilities for neutron scattering research and for providing outside-user scientists with office space and conference room facilities.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer:

Budget Authority in Thousands

Item	1981	1982	1983	1984	1985
Operations	$5.762	$6.599	$6.813	$7.467	$8.986
BES - Nuclear Sciences	3,494	3,798	5,590	6,150	7,820
BES - Materials Sciences	781	918	0	103	32
Isotope Sales Credits	779	842	644	805	726
MFE-ER	146	400	0	0	0
BER-ER	182	200	0	0	0
GCR-NE	182	130	100	0	0
Other-Misc	198	311	479	409	408
In-House Research	3.894	3.602	3.911	4.307	4.515
BES - Material Sciences	1,894	1,602	1,868	2,190	2,370
MFE-ER	1,200	1,350	1,460	1,617	1,545
GCR-NE	800	650	583	500	600
Out-of-House Research*	600	700	950	720	1.540
Other Operating Expense	0	0	0	0	0
Capital Equipment	234	654	863	848	532
BES - Nuclear Sciences	152	484	521	523	507
BES - Material Sciences	82	170	63	128	25
Japan	0	0	279	197	0
AIP - BES	0	0	0	0	300
General Plant Project - MFE-ER	0	0	0	475	600
In-House Energy Management	0	0	0	0	0
Other Construction	0	0	0	0	0
TOTAL COST	$10.490	$11.555	$12.729	$14.444	$16.798

Note: These amounts do not include Small Angle Scattering.

* The research is funded by sources in NSF, DOD, Other DOE, Industry, etc., and are obtained by the institutions doing the research and is usually not known by ORNL. In addition, research outside ORNL that depends on the availability of transplutonium isotopes produced at HFIR-TRU is funded by the BES Nuclear Sciences Program (approximately $4.5 M in 1983) and the DOE Office of Defense Programs (approximately $2 M).

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer: NEUTRON SCATTERING

Funding by other than DOE (Operating and Equipment):

Budget Authority in Thousands

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
U.S.-Japan Program	0	$360	$360	$396	$220
The above amounts include equipment furnished by Japan that is not included in Question 6 amounting to:		(230)	(50)	(130)	0
U.S.-Japan Program in MFE*	0	0	0	0	476
Isotope Production**	781	918	644	805	726

* Under a U.S./Japan collaborative agreement, the Japanese funds will be received by DOE Headquarters and funded to ORNL as DOE programmatic funds.

** Included in Question 6.

8. **For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.**

Answer: NEUTRON SCATTERING

Full-time Equivalents (FTE's)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Solid State Division	11.5	12.0	12.0	13.0	14.5
Japanese	0	0	2.0	2.0	2.0
Ames	3.0	3.0	3.0	3.0	3.0
Chemistry Division	3.0	3.0	3.0	3.0	3.0
	17.5	18.0	20.0	21.0	22.5

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
IRRADIATIONS					
Metals & Ceramics Division	12.0	12.0	12.0	12.0	12.0
REACTOR OPERATION*					
Operations Division	28.1	28.5	28.0	28.0	28.0
Support Divisions (P&E, I&C etc.)	16.0	16.0	16.5	19.4***	16.0
Laboratory Protection**	3.0	3.0	3.0	3.0	3.0

* Total staffing levels.
** Round-the-clock guard protection (not included in FTP/A).
*** Additional manpower for beryllium changeout.

9. **What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?**

Answer: NEUTRON SCATTERING

Neutron scattering facilities have had and continue to have full utilization. Full utilization is defined as utilization for research during 100% of the time that the HFIR is operating at full power. The HFIR is operating at full power approximately 93% of the time each year.

IRRADIATIONS

The premium neutron flux irradiation facilities are utilized approximately 95% of the time.

10. **For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?**

Answer: NEUTRON SCATTERING

During the period from FY 1981 to FY 1985, it is estimated that approximately 80 experiments were started and completed each year, except for the period that the facilities were removed from the reactor in FY 1984 to permit replacement of the beryllium reflector. The total number during this 5-year period is estimated to be about 350. This includes both in-house research and collaborative research by users.

FUSION ENERGY RESEARCH IRRADIATIONS

Forty HFIR capsules have been installed since 1981, and 32 will have been removed by 1985.

MISCELLANEOUS IRRADIATIONS

It is estimated that during the period approximately 18 experiments involving gas-cooled reactor and other programs will have been completed.

11. What is this facility's user policy?

Answer: The neutron scattering facilities are available to all scientists from other scientific organizations on a no-charge basis for research that is published in the open literature. Proprietary research can be performed through appropriate arrangements at full cost recovery.

The irradiation programs sponsored by ER are given first priority for reactor usage. DOE programs other than ER are given second priority, followed by other government programs and non-government programs, respectively.

12. For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?

Answer: NEUTRON SCATTERING

None.

13. What is the mechanism by which specific research proposals for experiments at the facility are considered?

Answer: NEUTRON SCATTERING

Research proposals are submitted in writing to the secretary of the Users' Program. The proposals are reviewed by a committee, and experimental time is allocated on the basis of scientific merit. Research can also be scheduled informally as collaborative research through interactions with interested members of the ORNL staff.

IRRADIATIONS

Plans for experimental irradiations must be submitted to the HFIR management for each capsule.

14. How many research proposals have been submitted over the past five years, and how many of these have been approved?

Answer: NEUTRON SCATTERING

The Users' Program has operated on a formal basis since January 1982. Since that time, approximately 80 proposals have been submitted for neutron scattering research; about 95% have been approved. In addition, many other potential proposals were discussed informally with staff members and discouraged, because the use of neutron scattering techniques would not have been appropriate.

IRRADIATIONS

Forty experimental plans for experimental irradiations have been submitted and approved.

15. How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?

Answer: About 40 different university facility members and students have used the neutron scattering facilities over the past five years. Many were repeat users during this period with an average number of about 20 university personnel/year.

NOTE: University users of the National Center for Small Angle Scattering Research are not included here. (110 university scientists used NCSASR facilities during this period.)

16. How many industrial researchers have utilized the facility over the past five years?

Answer: One industrial researcher has used the neutron scattering facilities over the past five years.

NOTE: Industrial users of the National Center for Small Angle Scattering Research are not included here. (31 industrial scientists used NCSASR facilities during this period.)

17. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer: About 40 foreign researchers have used the neutron scattering facilities over the past five years. Several of these researchers used the facilities for more than one experiment during this period.

NOTE: Users of the National Center for Small Angle Scattering Research from foreign institutions are not included here. (There were approximately 20 such users of NCSASR facilities during this period.)

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: Five researchers from other agencies have utilized the neutron scattering facilities over the past five years. Most of these researchers used the facilities several times during this period.

NOTE: Users of the National Center for Small Angle Scattering Research from other agencies are not included here. (There were 39 such users of NCSASR facilities during this period.)

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: NEUTRON SCATTERING

The existing neutron scattering spectrometers are being upgraded at an approximate cost of $100K/yr through FY 1985. We also are making plans to begin construction in FY 1985 of a new high-resolution diffractometer for structural and diffuse scattering studies that will incorporate position sensitive detectors for obtaining data at high rates. The estimated cost of this facility is $500K.

20. Please provide a copy of the facility's latest annual report.

Answer: Annual reports are not normally produced, but quarterly reports are. The latest quarterly report is attached as are excerpts from a brochure describing the HFIR neutron scattering facilities.

ORNL/TM-9051

Contract No. W-7405-eng-26

Operations Division

HIGH FLUX ISOTOPE REACTOR QUARTERLY REPORT
APRIL THROUGH JUNE, 1983

T. L. Dahl and K. H. Poteet

Sponsor: J. H. Swanks, Director
Operations Division

Date Published: February 1984

NOTICE This document contains information of a preliminary nature.
It is subject to revision or correction and therefore does not represent a final report.

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830
operated by
UNION CARBIDE CORPORATION
for the
DEPARTMENT OF ENERGY

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HIGH FLUX ISOTOPE REACTOR QUARTERLY REPORT
APRIL THROUGH JUNE, 1983

T. L. Dahl and K. H. Poteet

SUMMARY

Routine reactor operation with four end-of-cycle shutdowns and one unscheduled shutdown resulted in an on-stream time of 91.4% for the quarter. The outer control plates were replaced and a semiannual core component inspection was made.

OPERATIONS

Basic operating data for the quarter are listed in Table 1.

Table 1. HFIR basic operating data
(April 1 - June 30, 1983)

	This quarter	Last quarter	Year to date
Total energy, MWd	8220	8216	16,436
Average power, MW/operating h	99.9	99.9	99.9
Time operating, %	90.5	91.4	91.0
Reactor availability, %	91.4	91.5	91.4
Reactor water radioactivity, $\frac{c/min}{ml}$(av)	260,000	228,000	
Pool water radioactivity $\frac{c/min}{ml}$(av)	61	64	

The starting and ending dates for Cycles 237, 238, 239, 240, and 241 are presented in Table 2.

Table 2. Cycles of operation

Cycle No.	Date started	Date ended	Accumulated power (MWd)
237	3/19/83	4/12/83	2112
238	4/13/83	5/4/83	2122
239	5/6/83	5/27/83	2123
240	5/28/83	6/18/83	2122
241	6/21/83	In progress	984

The status of the HFIR fuel and control-plate inventory is indicated in Table 3.

Table 3. HFIR material inventory

Item	This quarter	Last quarter
New fuel elements placed in service	4	4
New fuel elements available for use	10	14
Spent fuel elements on hand	13	15
Spent fuel elements shipped	6	0
New sets of shim plates placed in service	0	0
New sets of shim plates available for use	4	4

SHUTDOWNS

There were four end-of-cycle shutdowns and one unscheduled shutdown for a total downtime of 208.101 hours. Table 4 gives further details.

Table 4. Description of HFIR shutdowns

Date	Downtime (hr)	Remarks
		Scheduled
4/12/83	33.483	Fuel cycle 237 was completed at 6:51 AM. A total power generation of 2112 MWd was obtained on fuel element 236 O&I.
5/4/83	26.067	Fuel cycle 238 was completed at 11:06 AM. A total power generation of 2122 MWd was obtained on fuel element 237 O&I.
5/27/83	33.234	Fuel cycle 239 was completed at 7:05 AM. A total power generation of 2123 MWd was obtained on fuel element 238 O&I.
6/18/83	53.317	Fuel cycle 240 was completed at 10:06 PM. A total power generation of 2122 MWd was obtained on fuel element 239 O&I. The shutdown was extended to inspect the primary heat exchanger tube baffles.
		Unscheduled
4/5/83	62.000	A TVA power interruption during an electrical storm resulted in primary pump shutdown and a reduction in reactor power to <10 MW. Xenon buildup precluded return to power.

PLANT MAINTENANCE

Maintenance and changes in the various systems are listed in Table 5.

Table 5. Process systems - maintenance and changes

Date	Component	Remarks
		Primary system
5/13/83	Valve	The exit valve, HCV-124, of the west primary demineralizer anion column failed to open. A new diaphragm was installed.
		Miscellaneous
5/9/83	Filters	The final absolute filters in the west SBHE filter compartment were replaced after failing the DOP efficiency test.
5/19/83	Crane brake	The 50-ton crane brake was replaced because of excessive wear.

INSTRUMENTATION AND CONTROLS

Maintenance and changes in the various instrumentation systems are listed in Table 6.

Table 6. Instrumentation - maintenance and changes

Date	Component	Remarks
4/8/83	Fission chamber	A faulty fission chamber servo motor amplifier was replaced in channel No. 1.
6/3/83	Decade scaler	A faulty decade scaler module in wide range counting channel No. 1 was replaced.
6/19/83	Magnet	Number 4 magnet was replaced with a spare because of a high drop current.

SYSTEM SURVEILLANCE TESTS AND RESULTS

Vessel Head Studs

The accumulated number of tensioning cycles on the reactor vessel head studs is presented in Table 7. These studs were designed for a fatigue life of 40 cycles loading due to tensioning of the bolts and 730 full-pressure 6.9-MPa (1000-psig) cycles. Installation of new reactor vessel head studs was completed in June 1972. The numbers in Table 7 represent the maximum cycles to which any new stud has been exposed.

Table 7. Vessel head stud-tensioning cycles

	This quarter	Last quarter	Total to date
Head bolts tensioned	0	0	6
10.3 MPa (1500 psig)	0	0	0
6.5 MPa (950 psig)	0	0	7
5.2 MPa (750 psig)	4	5	131
4.5 MPa (650 psig)	0	0	117

Stack Filters

Stack filtering systems in the special building hot exhaust (SBHE) and hot off-gas (HOG) systems were tested for particulate and iodine removal efficiency. Results of the most recent test are tabulated in Table 8.

Table 8. Particulate and iodine removal efficiency

Filter bank	Elemental iodine				Filter Position	Particulate retention			
	Last test		Previous test			Last test		Previous test	
	Date	Eff.,%	Date	Eff.,%		Date	Eff.,%	Date	Eff.,%
SBHE, west	1/11/83	99.98	4/20/82	99.98	South	4/21/83	99.99	9/28/82	99.98
					North	5/9/83	99.99	9/28/82	99.99
SBHE, center	2/1/83	99.61*							
	3/10/83	99.99	6/2/82	99.99	South	4/21/83	99.99	3/12/82	99.99
					North	4/21/83	99.99	3/12/82	99.99
SBHE, east	1/13/83	99.90	4/22/82	99.96	South	4/21/83	99.99	9/28/83	99.98
					North	4/21/83	99.99	9/28/83	99.98
HOG, west	2/3/83	99.99	5/11/82	99.99					
HOG, center	2/15/83	99.93	5/25/82	99.99					
HOG, east	2/17/83	99.91	5/27/82	99.98					

*Test results are less than minimum ORNL Standards. Charcoal was replaced and retested on 3/10/83. It was out of service during the interim.

Summary of Surveillance Tests

Table 9 is a tabulation of the completion dates of the surveillance tests required by the Technical Specifications. This table contains all the surveillance tests scheduled for frequencies of one month or longer. Other surveillance requirements which will not be reported are satisfied by the routine completion of daily and weekly check sheets, startup checklists, hourly data sheets, the operating logbooks, and miscellaneous quality assurance tests.

REVISIONS TO THE HFIR OPERATING MANUAL

There were no revisions made to the operating manual during the quarter.

UNUSUAL OCCURRENCES

There were no unusual occurrences this quarter.

REACTOR EXPERIMENTS

Experiment Facilities

Assignment of the various HFIR experiment facilities is tabulated in Table 10.

HFIR Target Loading

A description of the HFIR target loading for each of the operating cycles this quarter is presented in Figs. 1, 2, 3, 4, and 5.

Table 9. Summary of surveillance tests

Test	Most recent test	Previous test	Previous test
	Annual tests		
Count rate channel A calibration	10/1/82	2/2/82	9/3/81
Count rate channel B calibration	10/1/82	2/4/82	9/4/81
Count rate channel C calibration	10/1/82	2/18/82	9/10/81
Normal-emergency systems	1/6/83	9/21/82	6/23 82
Poison injection system	11/19/82	11/30/81	12/15/80
Pressurizer pump high-pressure cutoff	9/22/82	10/15/81	10/6/80
Pressure relief valves	2/22/83	3/24/82	5/21/81
Pressure vessel head studs	2/22/83	3/24/83	5/21/81
Radiation block valve test	11/19/82	11/30/81	12/15/80
Reactor bay in-leakage test	10/27/82	11/30/81	12/15/80
Reactor components	2/22 83	9/7/82	3/24/82
Safety channel A calibration	1/11/83	3/2/82	5/27/81
Safety channel B calibration	1/12/83	3/3/82	5/27/81
Safety channel C calibration	1/13/83	3/9/82	5/27/81
Servo channel A calibration	6/8/83	9/16/82	1/5/82
Servo channel B calibration	6/8/83	9/16/82	1/5/82
Servo channel C calibration	6/8/83	9/16/82	1/5/82
Speed of shim and regulating drives	2/22/83	3/24/82	5/21/81
Switchgear battery load test	5/5/83	6/23/82	9/17/81
	Semiannual tests		
Main pump low-pressure cutoff	5/5/83	11/19/82	6/23/82
Pony motor battery E	5/4/83	10/31/82	7/17/82
Pony motor battery F	6/18/83	2/21/83	11/18/82
Pony motor battery G	3/16/83	12/12/82	9/6/82
Pony motor battery H	5/27/83	1/5/83	9/30/82
Radiation monitoring equipment	1/13/83	7/27/82	3/10/82
SBHE filter efficiency	1/31/83	6/10/82	3/12/82
	Monthly tests		
Cadmium nitrate tests	6/18/83	5/21/83	4/16/83
Diesel run test, No. 1	6/14/82	5/17/83	4/12/83
Diesel run test, No. 2	6/14/82	5/17/83	4/12/83

Table 10. Experiment facility assignment

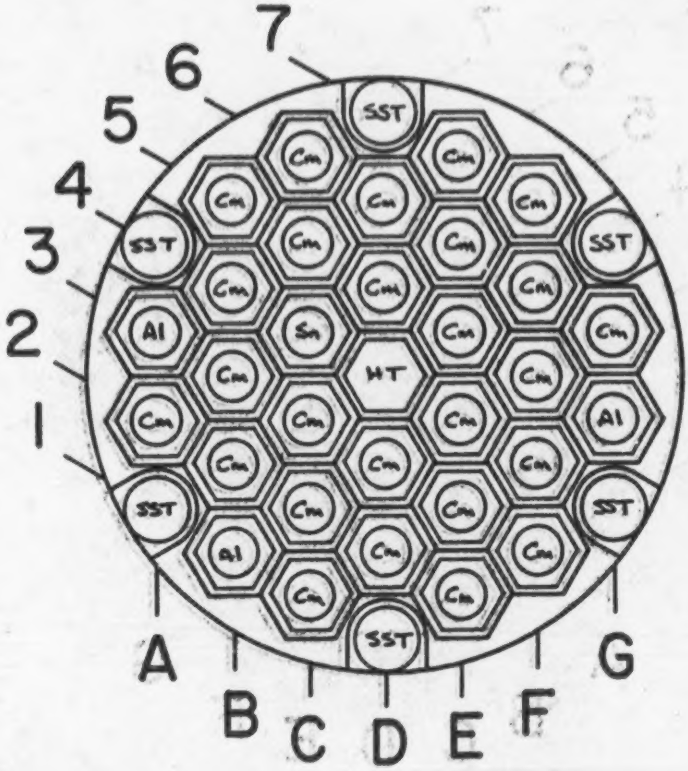
Facility	Description	Division
PTP-A1	Materials studies	Fusion Energy
PTP-A4	Materials studies	Fusion Energy
PTP-D1	Materials studies	Fusion Energy
PTP-D7	Materials studies	Fusion Energy
PTP-G4	Materials studies	Fusion Energy
PTP-G7	Materials studies	Fusion Energy
RB-1	Isotope production	Operations
RB-2	Isotope production	Operations
RB-3	Isotope production	Operations
RB-4	Isotope production	Operations
RB-5	Materials studies	Fusion Energy
RB-6	Isotope production	Operations
RB-7	Materials studies	Fusion Energy
RB-8	Isotope production	Operations
CR-1	Isotope production	Operations
CR-2	Isotope production	Operations
CR-3	Isotope production	Operations
CR-4	Isotope production	Operations
CR-5	Isotope production	Operations
CR-6	Isotope production	Operations
CR-7	Isotope production	Operations
CR-8	Isotope production	Operations
VXF-1	Isotope production	Operations
VXF-3	Isotope production	Operations
VXF-4	HFIR corrosion specimen	Operations
VXF-5	Isotope production	Operations
VXF-7	Pneumatic tube	Analytical Chemistry
VXF-9	Isotope production	Operations
VXF-11	Isotope production	Operations
VXF-13	Isotope production	Operations
VXF-15	Isotope production	Operations
VXF-18	Isotope production	Operations
VXF-20	Isotope production	Operations
VXF-22	Isotope production	Operations
HB-1	Neutron diffractometer	Solid State
HB-2	Neutron diffractometer	Chemistry
HB-3	Neutron diffractometer	Solid State
HB-4	Neutron diffractometer	Solid State

HFIR TARGET LOADING

CYCLE NO. 238

DATE 4/13/83

ORNL/DWG. 84-7159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Cm
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Cm
Cm
SST
A
B
C
D
E
F
G

TARGET TYPE	NUMBER
PLUTONIUM (Pu)	
CURIUM (Cm)	26
STAINLESS STEEL (SST)	6
GRAPHITE (C)	
ALUMINUM (Al)	3
HYDRAULIC TUBE (HT)	1

Fig. 1.

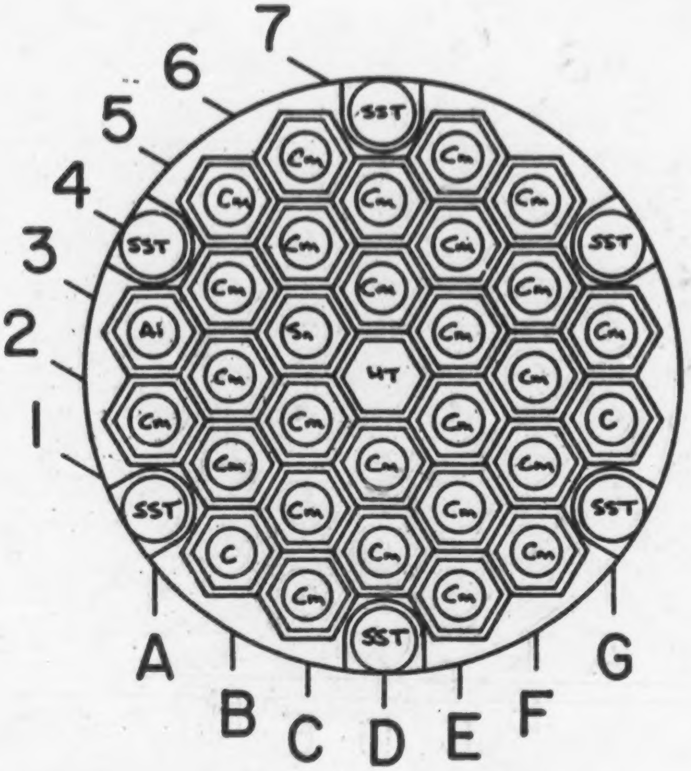
UCN-12912
(3 1-78)

HFIR TARGET LOADING

CYCLE NO. 239

DATE 5/6/83

ORNL/DWG. 84-7160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SST
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SST
C
Cm
Cm
Cm
Cm
SST
A
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C
D
E
F
G

TARGET TYPE	NUMBER
PLUTONIUM (Pu)	
CURIUM (Cm)	26
STAINLESS STEEL (SST)	6
GRAPHITE (C)	2
ALUMINUM (Al)	1
HYDRAULIC TUBE (HT)	1

Fig. 2.

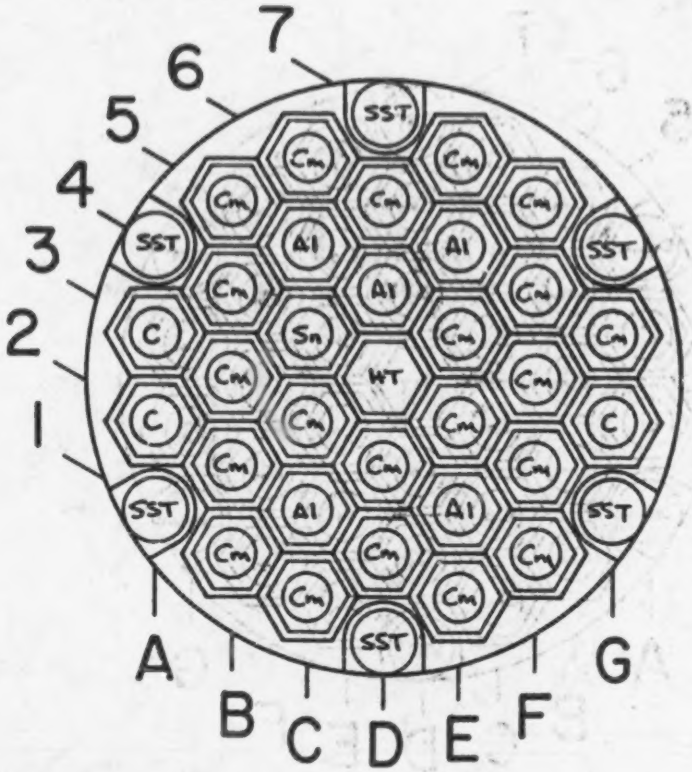
UCN-12912
(3 1-78)

HFIR TARGET LOADING

CYCLE NO. 240

DATE 5/28/83

ORNL/DWG. 84-7161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Sn
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Cm
SST
Al
Al
SST
Cm
Cm
Cm
Cm
Cm
SST
A
B
C
D
E
F
G

TARGET TYPE	NUMBER
PLUTONIUM (Pu)	
CURIUM (Cm)	21
STAINLESS STEEL (SST)	6
GRAPHITE (C)	3
ALUMINUM (Al)	5
HYDRAULIC TUBE (HT)	1

Fig. 3.

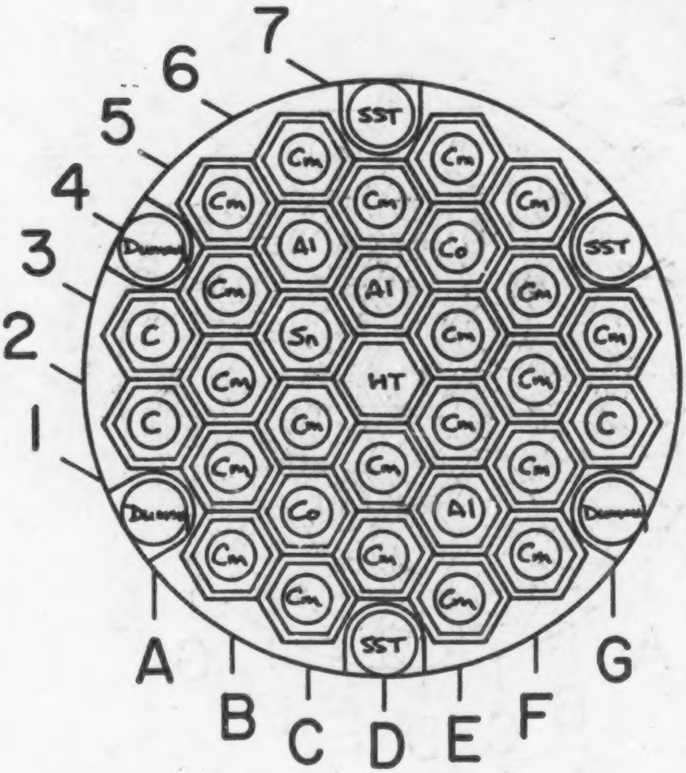
UCN-12912
(3 1-78)

HFIR TARGET LOADING

CYCLE NO. 241

DATE 6/20/83

ORNL/DWG. 84-7162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Sn
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Cm
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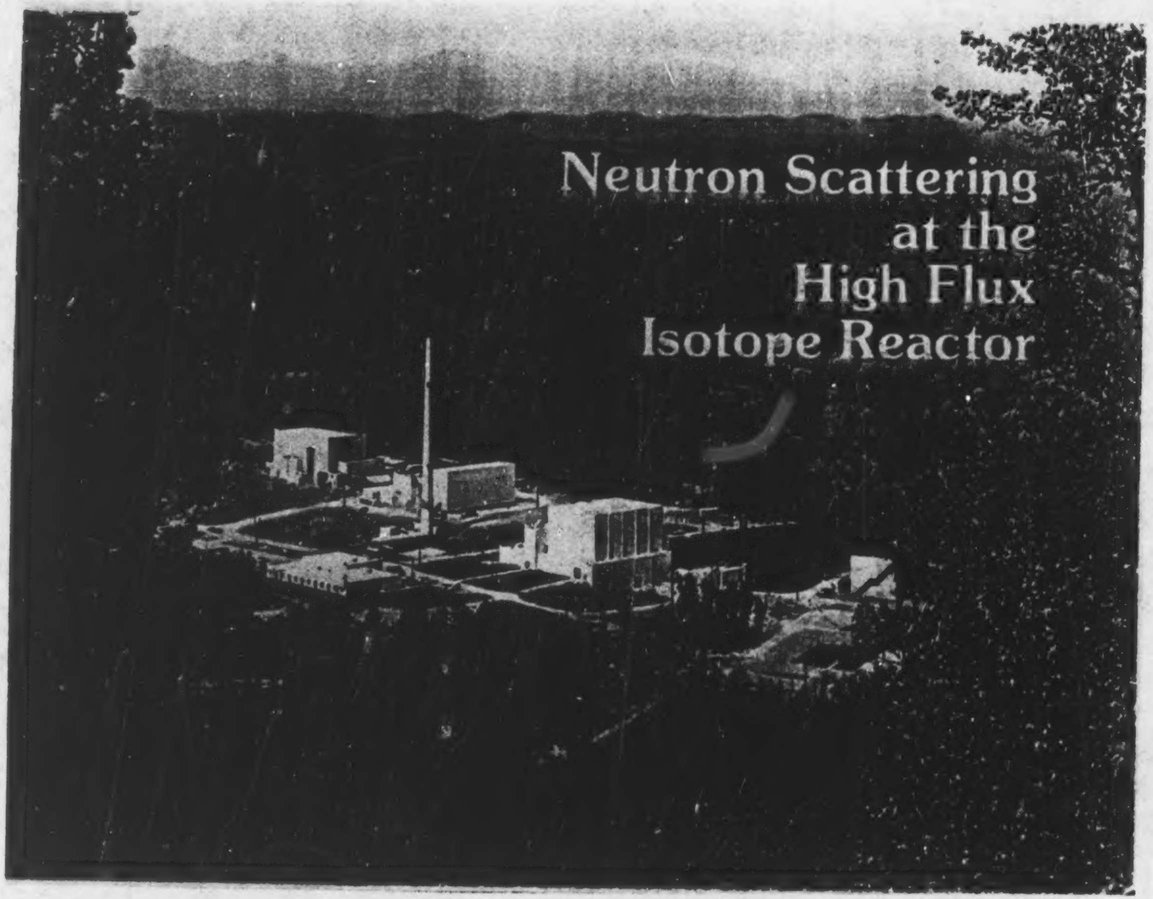
Cm
Dummy
Co
Al
Dummy
Cm
Cm
Cm
Cm
Cm
SST
A
B
C
D
E
F
G

TARGET TYPE	NUMBER
PLUTONIUM (Pu)	
CURIUM (Cm)	21
STAINLESS STEEL (SST)	3
GRAPHITE (C)	3
ALUMINUM (Al)	6
HYDRAULIC TUBE (HT)	1

Fig. 4.

UCN-12912
(3 1-78)


Neutron Scattering
at the
High Flux
Isotope Reactor

Preface

This booklet describes the neutron scattering facilities at the High Flux Isotope Reactor at the Oak Ridge National Laboratory. These facilities, which have been constructed by and operated with support from the Department of Energy, are available for use by outside scientists on problems of high scientific merit. This booklet, which should serve as a source of useful information for visitors and users of the neutron scattering facilities, was prepared by H. A. Mook of the Solid State Division.

R. M. Moon
Solid State Division
June 1, 1981

The High Flux Isotope Reactor

Since attaining its design power of 100 MW in September 1966, a little over five years from the beginning of construction, the High Flux Isotope Reactor (HFIR) has achieved a record of operation time unsurpassed by any other reactor in the United States. The HFIR is a beryllium-reflected, light-water-cooled and -moderated, flux-trap reactor with a design power level of 100 MW. It burns 93%-enriched ^{235}U fuel placed in aluminum-clad plates. A fuel cycle (the lifetime of a fuel assembly) is about 23 days. Although the main purpose of the reactor is to produce research quantities of transplutonium elements, its high flux makes it an excellent source of neutrons for neutron scattering experiments.

The reactor core is composed of a series of concentric annular regions, each about 60 cm high. A 13-cm-diam hole in the center of the core is used to irradiate target rods to produce transplutonium isotopes. The fuel is placed in two concentric cylinders in the form of curved fuel plates. The inner one has an inside diameter (ID) of 13 cm and an outside diameter (OD) of 27 cm; the outer element has an ID of 28 cm and an OD of 45 cm. The 1.3-mm-thick fuel plates are curved so that they are parallel, and they provide a constant coolant-channel width. They are of complex sandwich-type construction with the fissile material held between thin plates of aluminum. A core loading is about 9.4 kg of enriched uranium. The fuel region is surrounded by a 30-cm-thick ring of beryllium, which acts as a neutron reflector. The whole assembly is immersed in water, which serves as a second reflector of effectively infinite thickness.

The control rods, two thin neutron-absorbing concentric cylinders that move vertically between the outer fuel element and the beryllium reflector, are operated by drive mechanisms located under the reactor. The neutron-absorbing material for the inner control cylinder is arranged so that reactivity is increased by downward motion. This cylinder is used for shimming and regulation; it has no safety function. The outer control cylinder has four separate sections, each with its own drive and safety release mechanism. Reactivity is increased as the outer plates are raised.

The entire reactor assembly is contained inside an 2.4-m-diam pressure vessel that is in a 5.5-m-diam tank filled with water. The top of the pressure vessel is 5.2 m below the water surface; the reactor center line is 3.2 m farther below. Adjacent to and connected with the reactor pool is a storage pool that is 5.5 m wide, 12.5 m long, and 6.1 m deep.

The reactor coolant (demineralized light water) is impelled by three vertical centrifugal pumps and flows through the reactor primary system at about 65,000 L/min. The normal system pressure of 4,500 kPa is provided by a nine-stage horizontal centrifugal pump. The coolant enters the primary system at 48°C and exits at 72°C. The heat removed is dissipated to the atmosphere by a conventional cooling tower.

The reactor is provided with four 10-cm-ID horizontal beam tube experimental facilities that extend outward from the reactor core at the midplane of the reactor. Beam tube HB-2 extends radially from the reactor center line with its inner end penetrating the permanent reflector. Beam tube HB-3, which extends tangentially from the core and is offset 27 cm from the reactor center line, also penetrates the permanent reflector. A third tube is aligned on a tangential line 39 cm from the reactor center line with both ends extending outward from the reactor so as to allow the installation of two individual facilities. The two ends of this tube are designated HB-1 and HB-4.

Provision has been made for the future installation of up to four engineering facilities to provide additional neutron beams for experiments. However, these engineering facilities have lower flux than

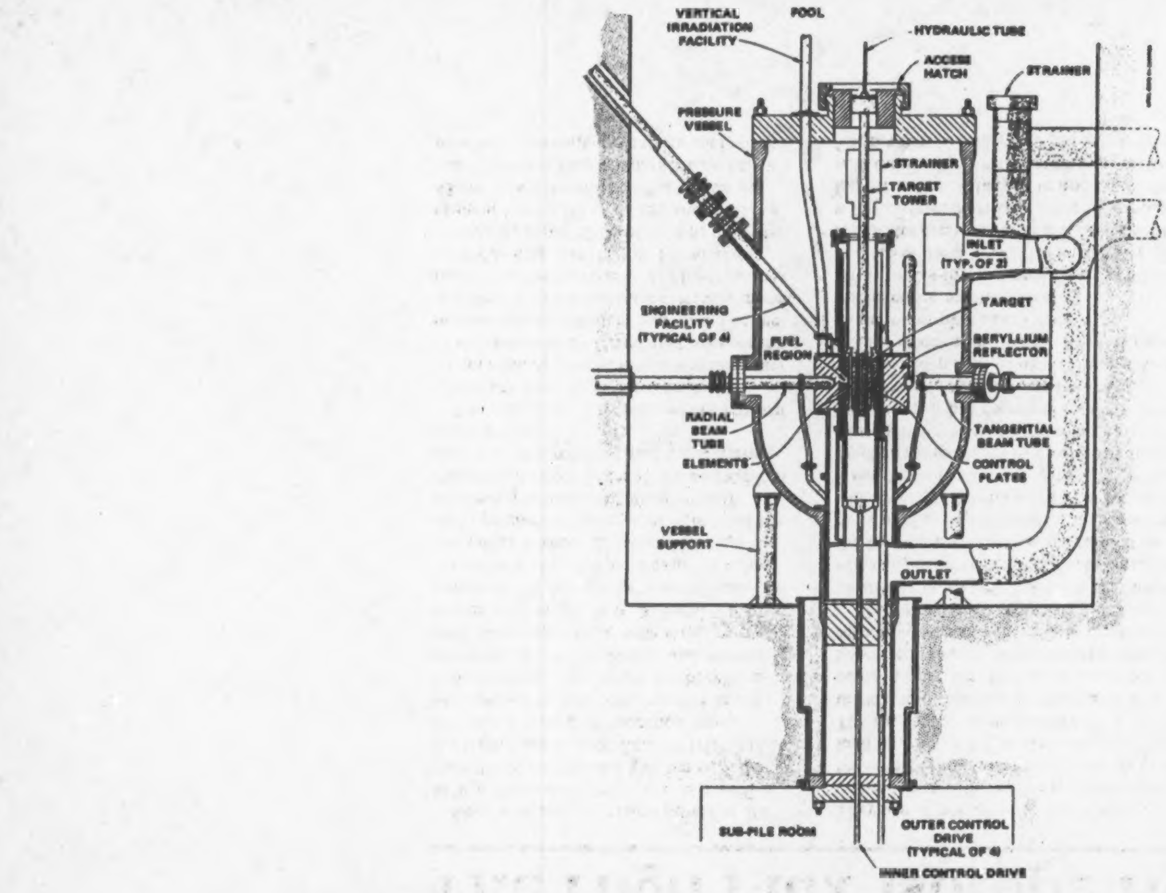

VERTICAL IRRADIATION FACILITY
POOL
HYDRAULIC TUBE
ACCESS HATCH
STRAINER
PRESSURE VESSEL
STRAINER
TARGET TOWER
INLET (TYP. OF 2)
TARGET
ENGINEERING FACILITY (TYPICAL OF 4)
FUEL REGION
BERYLLIUM REFLECTOR
RADIAL BEAM TUBE
TANGENTIAL BEAM TUBE
ELEMENTS
CONTROL PLATES
VESSEL SUPPORT
OUTLET
SUB-PILE ROOM
OUTER CONTROL DRIVE (TYPICAL OF 4)
INNER CONTROL DRIVE

Fig. 1. Vertical Section of Reactor Vessel.

the main beam tubes. The engineering facilities consist of 10-cm-OD tubes that extend downward into the reactor at an angle of 41° to provide access to flux at the outer periphery of the beryllium. The upper ends of the tubes terminate at the outer face of the pool wall in the experiment room, which is above the main beam room.

The schematic diagram of the reactor in Fig. 1 shows how the beam tubes enter the pressure vessel and end in the beryllium reflector. One of the engineering facility beam tubes can also be seen tilted upward from the reactor core. Figure 2 is a plan view of the reactor core that shows more clearly how the beam tubes enter the reflector. A scattering block of beryllium has been placed at the center line between beam tubes HB-1 and HB-4, effectively making them into two tangential tubes. The access holes in the beryllium reflector that may be used for irradiations are also shown. Figure 3 shows the flux distribution as a function of distance from the reactor center line. Note that the thermal flux peaks in the target irradiation region and in the beryllium reflector. The position of the end of the beam tubes in the beryllium is shown by the dashed line at about 33 cm. The thermal flux at the end of the beam tubes is above 10^{15} neutrons/cm^2 sec.

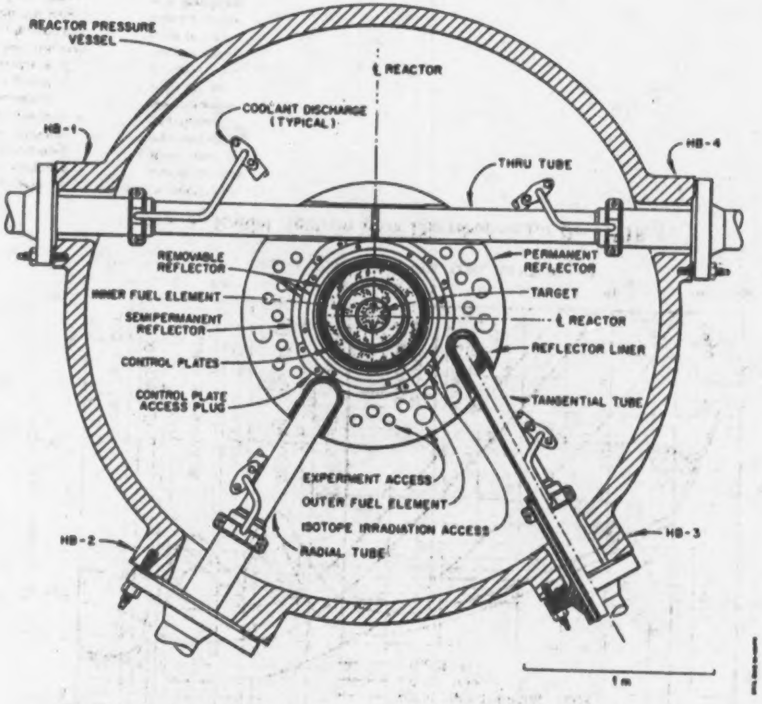

REACTOR PRESSURE VESSEL
℄ REACTOR
COOLANT DISCHARGE (TYPICAL)
HB-1
HB-4
THRU TUBE
REMOVABLE REFLECTOR
INNER FUEL ELEMENT
SEMIPERMANENT REFLECTOR
CONTROL PLATES
CONTROL PLATE ACCESS PLUG
PERMANENT REFLECTOR
TARGET
℄ REACTOR
REFLECTOR LINER
TANGENTIAL TUBE
EXPERIMENT ACCESS
OUTER FUEL ELEMENT
ISOTOPE IRRADIATION ACCESS
RADIAL TUBE
HB-2
HB-3
1 m

Fig. 2. Horizontal Midsection of the High Flux Isotope Reactor.

Reactor Parameters

Power	100 MW
Flux	5×10^{15} neutrons/cm^2 sec
Core type	Plates within concentric cylinders
Fuel	93%-enriched uranium
Fuel loading	9.40 kg ^{235}U
Fuel lifetime	23 d
Percent of time operating	91.5
Reactor vessel	Carbon steel, 6.1 m high, 2.4 m in diameter
Control rods	Concentric cylinders EuO-Al
Moderator	H_2O
Reflector	Permanent and removable Be sections
Coolant	H_2O, 65,000-L/min flow through vessel
Coolant temperature	48°C inlet, 72°C outlet
Average power density in core	2 MW/L
Experiment facilities	16 4-cm-diam vertical facilities 41 cm from core center line 6 7.3-cm-diam vertical facilities 48 cm from core center line 4 10-cm-ID horizontal beam ports: one beam radial to active core, one tangent to active core, and one penetrating entire reflector-vessel assembly; a Be scattering block placed in the center of this latter through-beam hole divides it into two separate beam lines 4 10-cm-OD engineering facilities at the outer periphery of Be reflector oriented at an angle 41° to the vertical and recessed a maximum of 5.8 cm into the permanent beryllium

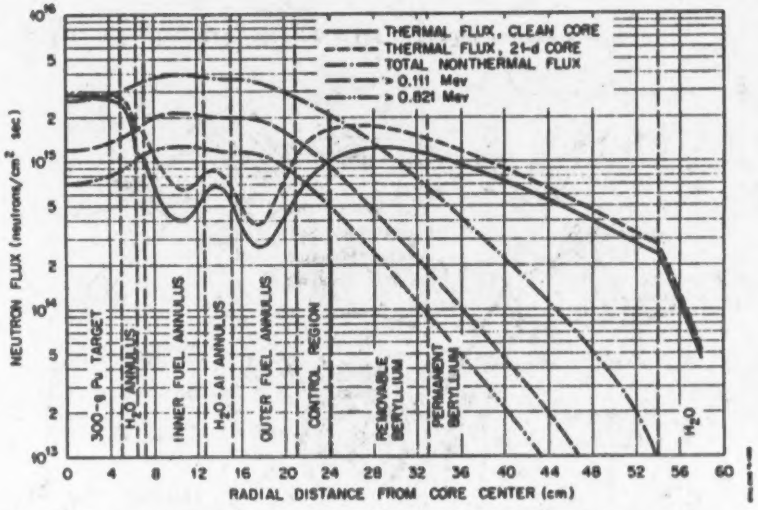


Fig. 3. Radial Neutron Flux Distribution for the HFIR.

Layout of Neutron Scattering Facilities

Figure 4 is an overall layout of the neutron scattering facilities on the main experiment floor. All the neutron scattering spectrometers are located on this floor except the National Small-Angle Scattering Facility, which is located on the first floor above this area. Each beam port has a main spectrometer that utilizes a large monochromator shield that can be rotated under computer control. This shield provides protection from the primary reactor beam and is 2.35 m in diameter and weighs approximately 38,000 kg. A system of wedges forms part of the shield and lifts out of the way of the primary beam while providing shielding in other directions. The minimum shielding in any direction through the monochromator shield is about 92 cm. The rotating monochromator shields at each beam port are identical even though the rest of the spectrometer may be quite different. At the HB-1 port, the main spectrometer using this rotating monochromator shield is a polarized beam spectrometer. At HB-2 and HB-3, triple-axis spectrometers use the large monochromator drum; at HB-4 the drum forms part of a time-of-flight spectrometer.

In addition to the large monochromator shield at each beam port there is provision for extracting a beam at a fixed angle from the primary beam. This side beam line is used in different ways for each beam port. At HB-1 it is used for a three-axis spectrometer; at HB-2 a diffractometer with a position-sensitive detector is installed in this position. At HB-3 the side beam is utilized by a small-angle scattering spectrometer, and at HB-4 a four-circle diffractometer utilizes this beam.

Figure 5 is an expanded picture of the HB-3 port showing how the two spectrometers are located. The primary beam passes through the monochromator for the small-angle scattering spectrometer, then through the wedge system, and is incident on the monochromator of the triple-axis spectrometer. The monochromator for the small-angle spectrometer, a thin slice of a perfect silicon single crystal, removes only a small number of neutrons from the primary beam so that essentially the full primary flux is available for the triple-axis spectrometer. A shutter is available to open and close the primary beam. The beam from the monochromator of the triple-axis spectrometer passes through a collimator and then is incident on the sample. Scattered neutrons from the sample pass through a collimator and are reflected from the analyzer into a BF_3 detector.

The silicon crystal for the small-angle spectrometer reflects neutrons through a collimator onto the sample located in the superconducting magnet. From there the beam is diffracted onto the analyzing crystal and into the detector.

We see that while two spectrometers share the same beam, they do not interfere with each other. Thus, although the HFIR has only four beam ports, these ports can support a wide variety of neutron scattering instrumentation. In fact, the HB-4 port supports three spectrometers: the time-of-flight spectrometer, the four-circle spectrometer, and the National Small-Angle Scattering Facility. These spectrometers work independently, each using a small wavelength slice from the primary beam. The operation of individual instruments is described in the following section.

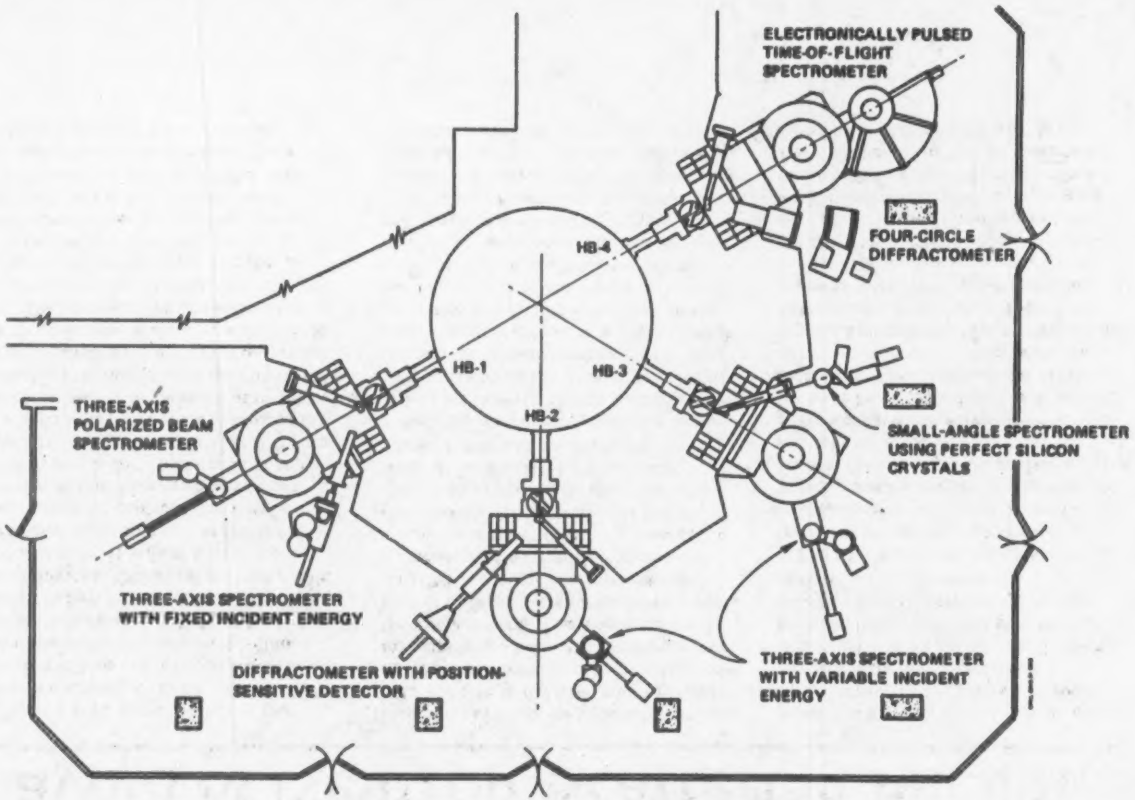

ELECTRONICALLY PULSED TIME-OF-FLIGHT SPECTROMETER
FOUR-CIRCLE DIFFRACTOMETER
HB-4
HB-1
HB-3
HB-2
THREE-AXIS POLARIZED BEAM SPECTROMETER
SMALL-ANGLE SPECTROMETER USING PERFECT SILICON CRYSTALS
THREE-AXIS SPECTROMETER WITH FIXED INCIDENT ENERGY
DIFFRACTOMETER WITH POSITION-SENSITIVE DETECTOR
THREE-AXIS SPECTROMETER WITH VARIABLE INCIDENT ENERGY

Fig. 4. Layout of the Neutron Scattering Facilities.

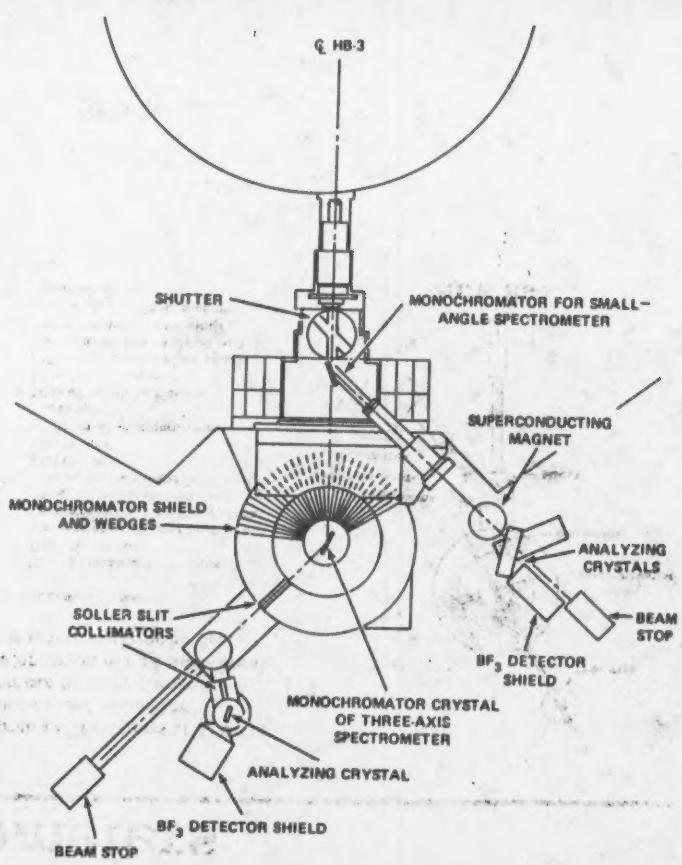

℄ HB-3
SHUTTER
MONOCHROMATOR FOR SMALL-ANGLE SPECTROMETER
SUPERCONDUCTING MAGNET
MONOCHROMATOR SHIELD AND WEDGES
ANALYZING CRYSTALS
BEAM STOP
SOLLER SLIT COLLIMATORS
BF3 DETECTOR SHIELD
MONOCHROMATOR CRYSTAL OF THREE-AXIS SPECTROMETER
ANALYZING CRYSTAL
BF3 DETECTOR SHIELD
BEAM STOP

Fig. 5. Spectrometers at the HB-3 Beam Port.

Neutron Spectrometers

HB-1 Spectrometer

The HB-1 spectrometer (Fig. 6) is generally used as a polarized beam spectrometer for elastic scattering studies, but it has all the capabilities of a three-axis spectrometer. This means that polarization analysis, as well as energy analysis, of the scattered beam from the sample is possible. The polarization state of the neutron beam is controlled by a radio-frequency flipping device that may be placed in either the incident or the scattered beam. Because the flipper is interfaced to the computer controlling the experiment, the polarization state can be changed at any time during the experiment. Usually the sample is placed in a superconducting magnet that provides a vertical field of up to 5 T. When a horizontal field is desired, an electromagnet is used. The incident neutron energy can be continuously varied by changing the monochromator angle $2\theta_m$. The (110) reflection from an ^{57}Fe(Si) crystal is used to produce the polarized beam. The spectrometer can be easily changed to unpolarized operation using a dual-crystal mount in the monochromator housing.

Spectrometer Parameters

$2\theta_m$	10 to 50° monochromator angle
$2\theta_d$	±120° detector angle
ϕ	Scattering angle, 90° maximum with superconducting magnet and vertical field, 60° maximum with electromagnet and horizontal field
ϕ	+180 to −180°
θ_A	+180 to −180°
Collimation	10′, 20′, or 40′ monochromator to sample 20′ or 40′ sample to analyzer
Beam size	2.5 by 3 cm maximum
Flux	2.57 × 10^6 neutrons/cm^2 sec polarized neutrons incident on sample with 40′ collimation at a wavelength of 1.04 Å. An ^{57}Fe monochromator-polarizer is used.

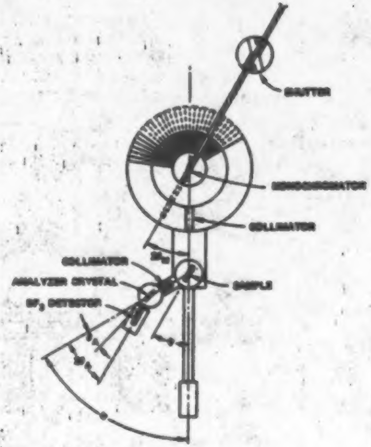


Fig. 6. HB-1.

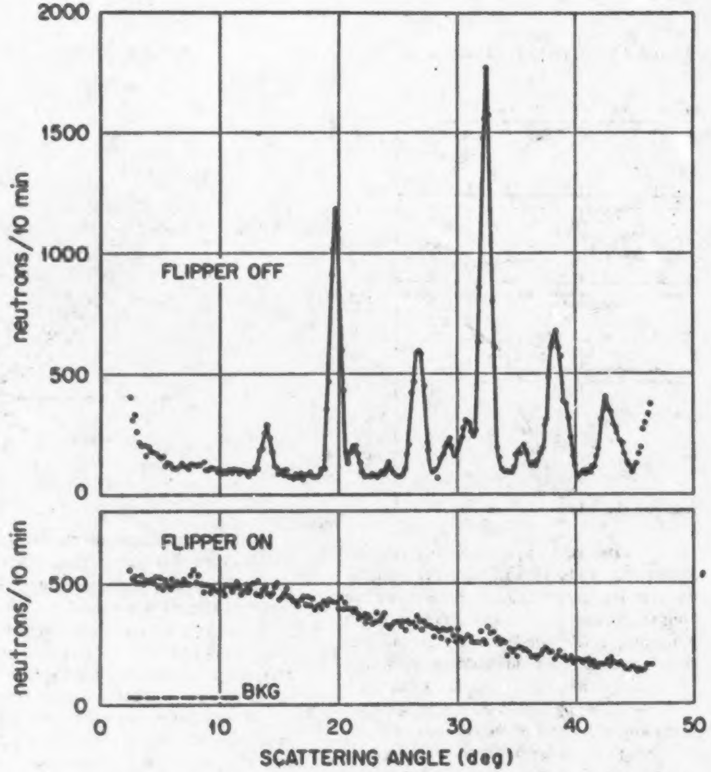


Fig. 7. Powder Diffraction Pattern of Gd_2O_3.

Figure 7 shows a powder diffraction pattern measured from 1.5 cm^3 of $^{160}Gd_2O_3$ at 293 K. Note that the non-spin-flip scattering measured with the flipper off shows the nuclear diffraction peaks, while the spin-flip scattering measured with the flipper on shows only the paramagnetic scattering.

HB-1A Spectrometer

The HB-1A spectrometer (Fig. 8) is a triple-axis spectrometer that uses a fixed incident energy generally set at 14.7 meV so that higher order contamination can be removed by a pyrolytic graphite filter. For this energy, a bent pyrolytic graphite crystal is used as a monochromator. Analyzing crystals are usually either pyrolytic graphite or beryllium, depending on the resolution desired. The detector is a ^{3}He detector mounted vertically so that a large vertical divergence of the scattered beam may be utilized if necessary.

Spectrometer Parameters

$2\theta_m$	Fixed, usually, E_o = 14.7 meV (λ = 2.353 Å)
$2\theta_A$	−100 to +100°
ϕ	−90 to 103°. This full range may not be available if the HB-1 spectrometer is positioned at large $2\theta_m$ values
ψ	−180 to +180°
θ_A	−180 to +180°
Collimation	10′ to 90′ before sample; 10′ to 90′ after sample
Beam size	5 by 3.75 cm maximum
Flux	9×10^6 neutrons cm^{-2} sec^{-1} at λ = 2.353 Å with 40′ collimation and a pyrolytic filter in the incident beam to eliminate higher order contamination

Figure 9 shows spin waves measured from ^{153}EuO at the (111) zone boundary at various temperatures. The crystal size was 10 × 10 × 2 mm, and the sample was made from europium enriched in the lower-neutron-absorbing isotope ^{153}Eu. The measurements show that rather well-defined spin wave excitations exist in EuO even above the Curie temperature T_c for the (111) zone boundary position. Counting times are about 40 min/point, and the temperature-independent background has been subtracted from the measurements.

HB-2 Spectrometer

The HB-2 spectrometer (Fig. 10) is a very flexible three-axis spectrometer. The incident energy can be made continuously variable by changing the $2\theta_m$ monochromator angle. Pyrolytic graphite, beryllium, or germanium are mainly used as monochromators, depending on the desired incident energy range. These same crystals are also used as analyzers. The detector is a vertical ^{3}He detector that can accept a large vertical divergence when necessary.

Spectrometer Parameters

$2\theta_m$	10 to 100°
$2\theta_A$	±110°
ϕ	+125 to −90°
ψ	−180 to +180°
θ_A	−180 to +180°
Collimation	10′ to 90′ before sample; 10′ to 90′ after sample
Beam size	5 by 3.75 cm maximum
Flux	$10^{[illegible]}$ neutrons cm^2 sec at λ = 2.353 Å and pyrolytic graphite used as a monochromator with a pyrolytic graphite filter used to eliminate higher order contamination and a collimation of 40′

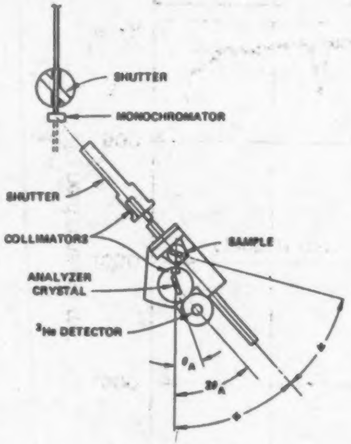

SHUTTER
MONOCHROMATOR
SHUTTER
COLLIMATORS
SAMPLE
ANALYZER CRYSTAL
^{3}He DETECTOR
θ_A
$2\theta_A$

Fig. 8. HB-1A.

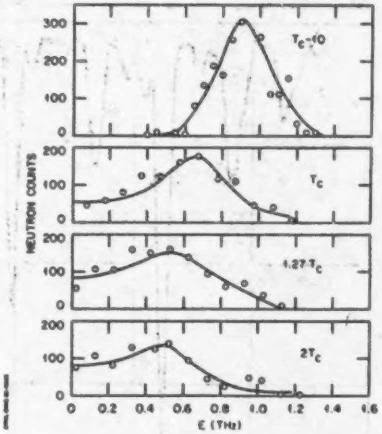


Fig. 9. Magnetic Excitations on EuO.

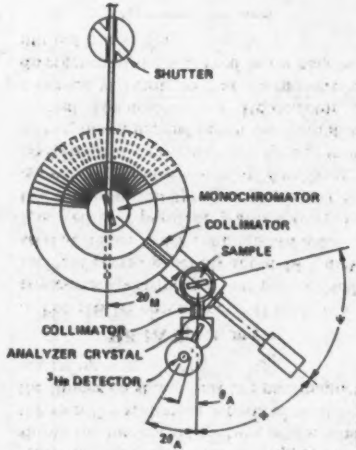

SHUTTER
MONOCHROMATOR
COLLIMATOR
SAMPLE
$2\theta_M$
COLLIMATOR
ANALYZER CRYSTAL
^{3}He DETECTOR
θ_A
$2\theta_A$

Fig. 10. HB-2.

Figure 11 shows the measured dispersion relation for transverse acoustic phonons in the [110] direction for a 5-cm^3 KCl crystal containing 1% CN$^-$ molecular impurities. These results show the temperature dependence of the coupling between these phonons and the librational modes of the CN . The experiment is very difficult because of the need for good energy resolution to measure a small energy splitting at low temperature, where the phonon-scattering cross section is small. An energy resolution of approximately 0.07 THz was obtained using a neutron energy of about 3.6 THz, 10′ collimation before and after the sample, and beryllium crystals for the monochromator and the analyzer. To obtain these data required approximately two weeks on the HB-2 spectrometer.

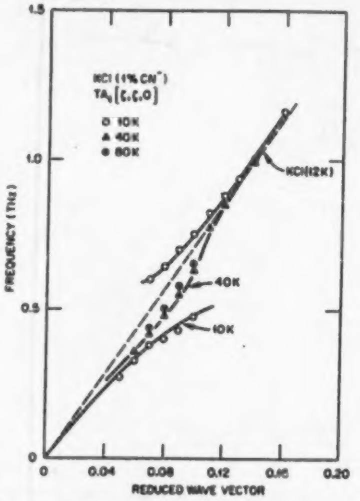


Fig. 11. Phonon Dispersion for KCl(CN).

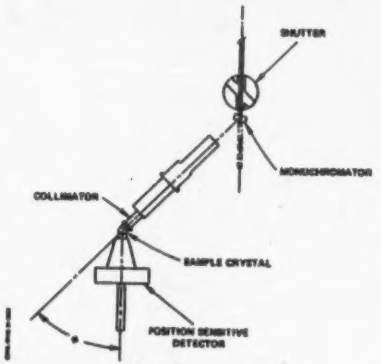


Fig. 12. HB-2A.

HB-2A Spectrometer

The HB-2A spectrometer (Fig. 12) is a diffractometer that uses a fixed incident neutron energy and a position-sensitive detector. The spectrometer is generally used with rather high incident neutron energies to measure the structure factor of liquids to high values of momentum transfer *Q*. The spectrometer can also be utilized as a high-data-rate powder diffractometer. Monochromating crystals are usually either germanium or beryllium. The present position-sensitive detector covers an angular range of 30°; however, it is expected that a larger detector will be installed.

Spectrometer Parameters

$2\theta_m$	45° fixed
ϕ	0 to 130° covered in 30° increments by a position-sensitive detector
Collimation	20′ to 1° before sample
Beam size	1 by 3.4 cm maximum
Flux	6.8×10^6 neutrons cm^{-2} sec^{-1} for λ = 0.89 Å using a germanium monochromator with the (422) reflection and a collimation of 20′

Figure 13 shows a measurement of the powder diffraction lines from a 2.1-cm^3 sample of nickel powder. The change in the symbol used in the plot shows when the position-sensitive detector was moved to cover a different value of momentum transfer. Note that a region of overlap exists for each time the detector was moved, and good agreement is obtained between the measurements made at different detector positions.

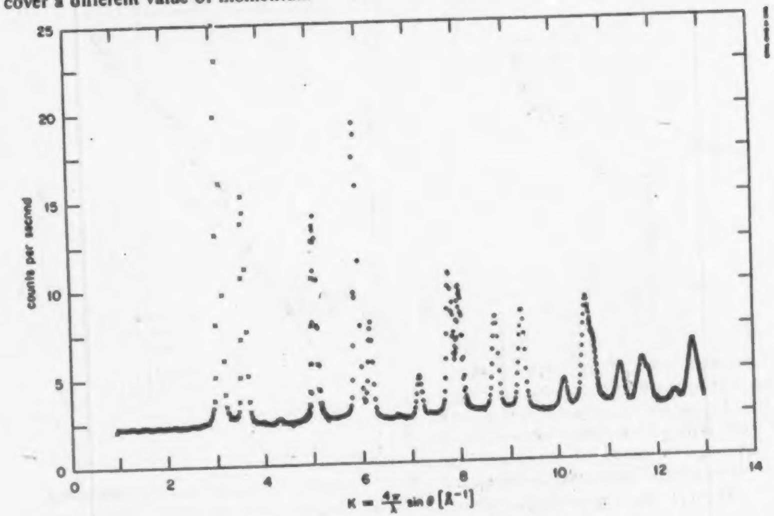


Fig. 13. Nickel Powder Diffraction Pattern.

HB-3 Spectrometer

The HB-3 spectrometer (Fig. 14) is a three-axis spectrometer similar to the HB-2 spectrometer. The incident energy is continuously variable by changing the $2\theta_m$ monochromator angle. Pyrolytic graphite, beryllium, or germanium are generally used as monochromator and analyzer crystals. The detector is a horizontally mounted BF_3 detector.

Spectrometer Parameters

$2\theta_m$	10 to 90°
$2\theta_A$	±110°
ϕ	−55 to +135°
ϕ	−180 to +180°
θ_A	−180 to +180°
Collimation	10′ to 90′ before sample; 10′ to 90′ after sample
Beam size	5 by 3.75 cm maximum
Flux	10^7 neutrons/cm^2 sec with beryllium 002 monochromator 40′ collimation and an incident wavelength of 1.4 Å 6.6×10^6 neutrons/cm^2 sec with beryllium 101 monochromator

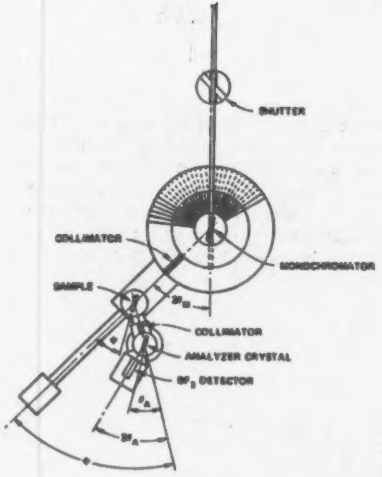

SHUTTER
COLLIMATOR
MONOCHROMATOR
SAMPLE
$2\theta_m$
COLLIMATOR
ANALYZER CRYSTAL
BF_3 DETECTOR
ϕ
θ_A
$2\theta_A$
ϕ

Fig. 14. HB-3.

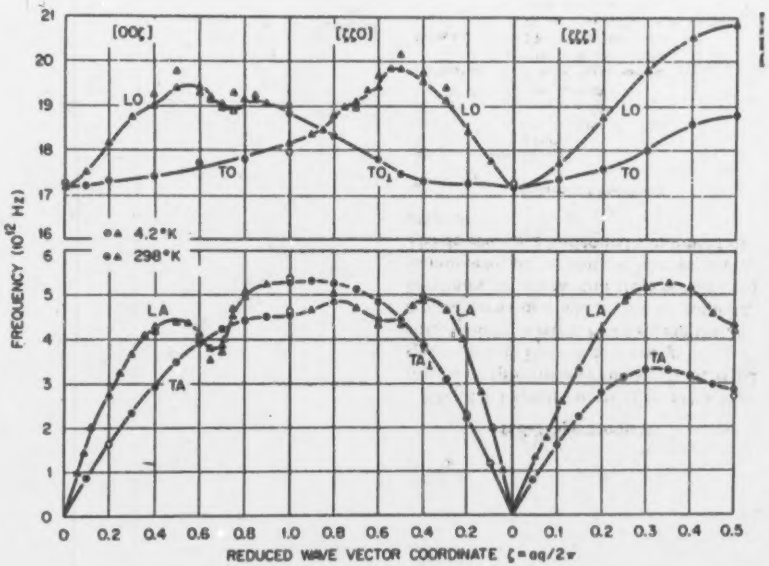


Fig. 15. Phonon Spectra of TaC.

Figure 15 shows the phonon spectra of TaC measured with the HB-3 spectrometer. The crystal size was about 0.5 cm^3, and the measurement took about two weeks. TaC is a superconductor at low temperatures, and anomalies in the phonon spectra are found that result from the large electron-phonon interaction.

HB-3A Spectrometer

The HB-3A (Fig. 16) is a small-angle scattering spectrometer that uses perfect silicon crystals to obtain high angular resolution. The angular resolution in the horizontal plane is very high, but the vertical resolution is poor, so the spectrometer is useful for looking at filamentary structures. This is the case for a fluxoid lattice aligned in the vertical direction by a magnet, and a number of interesting studies have been performed on superconductors using this instrument. The sample is usually placed in a superconducting magnet that can produce a uniform field of up to 1.2 T at the sample position.

Spectrometer Parameters

Resolution	4×10^{-5} Å^{-1}
Beam size	4 cm high by 2 cm wide maximum
Flux	10^4 neutrons/cm^2 sec at $\lambda = 2.6$ Å

Figure 17 shows the measurement of a fluxoid peak in niobium. Notice the very high resolution that results in a very clean separation of the fluxoid peak from the main unscattered beam. The counting rate of the fluxoid peak is quite high, around 500 counts/sec.

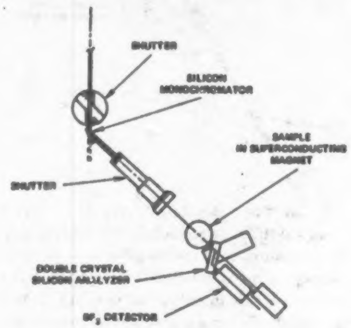

SHUTTER
SILICON MONOCHROMATOR
SAMPLE IN SUPERCONDUCTING MAGNET
SHUTTER
DOUBLE CRYSTAL SILICON ANALYZER
BF$_3$ DETECTOR

Fig. 16. HB-3A.

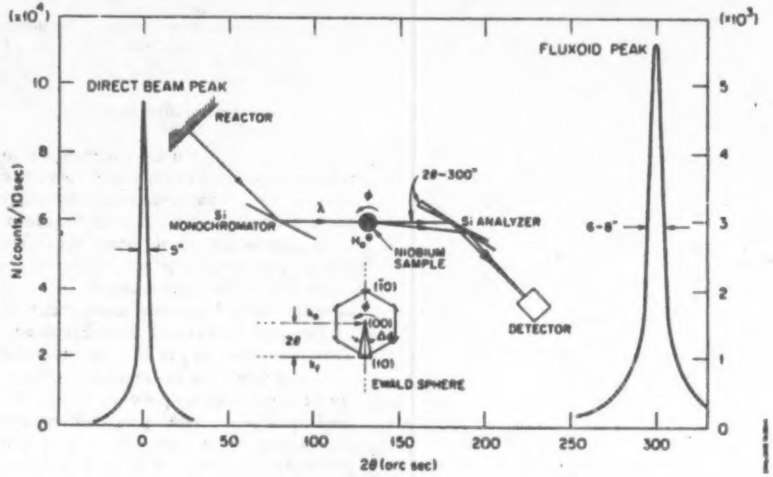


Fig. 17. Measurement of Fluxoid Lattice in Nb.

HB-4 Spectrometer

The HB-4 spectrometer (Fig. 18) is a very flexible time-of-flight spectrometer. The incident neutron energy can be made continuously variable by changing the $2\theta_m$ angle. The silicon monochromator is also used to pulse the neutron beam by being excited with high-power ultrasonic waves. The ultrasonic frequency is high, on the order of 10 MHz; therefore the time resolution is very good. Because the beam is pulsed electronically, a pulse can occur at any time and the cross-correlation technique can be used to give a high signal-to-noise ratio. Signal codes are stored in an on-line computer and can be of various lengths and duty cycles. The neutrons scattered from the samples are timed over a 1.5-m flight path and can be collected simultaneously in 70 ^{3}He detectors that can be placed at any position over a 10 to 130° angular range. The spectrometer can also be used as a polarized beam time-of-flight spectrometer in which the beam polarization is varied according to a pseudorandom code. This makes the spectrometer very useful for measuring magnetic excitations in ordered ferromagnetic systems because all phonon and elastic scattering can be avoided by use of the polarized beam.

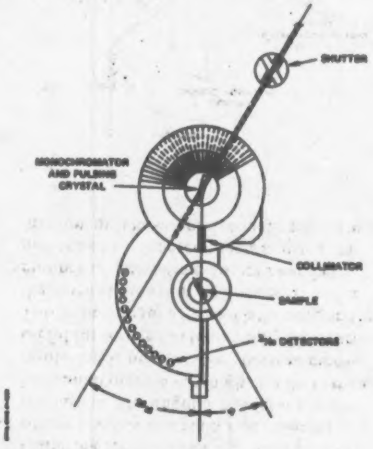


Fig. 18. HB-4.

Spectrometer Parameters

$2\theta_m$	10 to 90°
ϕ	0 to 130°
φ	−180 to +180°
Collimation	10′ to 90′ before sample; 20′ to open after sample
	70 detectors available and may be connected in any manner to 32 separate inputs to the data acquisition computer
Beam size	5 by 3.75 cm maximum
Flux	2.15 × 10^6 neutrons/cm^2 sec with a polarized beam from a ^{57}Fe monochromator and a collimation of 40′ for λ = 1.07 Å.

Figure 19 shows the crystal field levels measured in the superconductor $ErMo_6Se_8$. The sample was 1 cm^3 and counting time was 8 h.

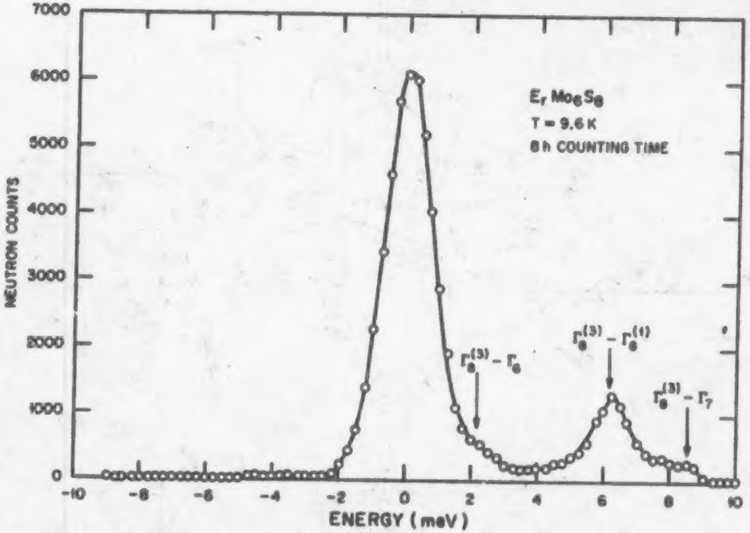


Fig. 19. Crystal Field Spectrum of $ErMo_6Se_8$.

HB-4A

The HB-4A (Fig. 20) is a four-circle diffractometer used for determining the crystal structure of single crystal samples. The spectrometer is fully computerized for the rapid measurement of a large number of Bragg reflections.

Spectrometer Parameters

Collimation	0.15° before sample
Beam size	5 mm square
Flux	2×10^6 neutrons cm^{-2} sec^{-1} from a beryllium monochromator set at a wavelength of 1.015 Å
Sample size	Normally 3 to 30 mm^3
Data rate	From 100 to 400 reflections per day
2θ maximum	130°

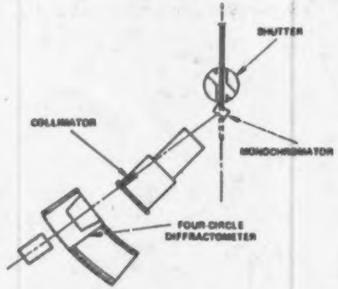


Fig. 20. HB-4A.

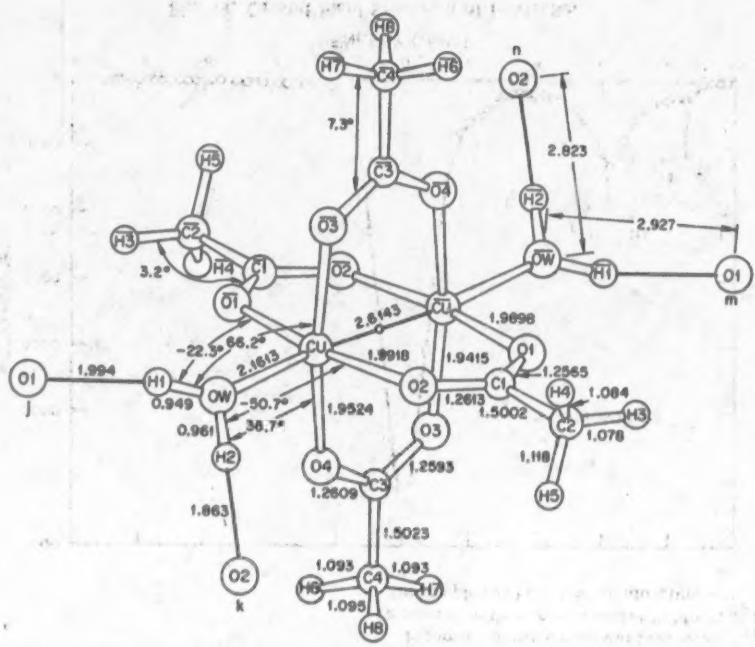

O1
j
1.994
H1
0.949
OW
0.961
H2
1.863
O2
k
-22.3°
66.2°
2.1613
-50.7°
38.7°
CU
2.6143
1.9918
1.9524
1.9415
1.9698
O4
1.2609
C3
1.2593
O3
1.5023
C4
1.093
1.093
1.095
H6
H7
H8
O2
C1
1.2613
1.5002
1.2565
O1
H4
1.084
C2
H3
1.078
1.118
H5
O̅1
C̅1
H̅4
C̅2
H̅3
H̅5
3.2°
O̅2
O̅3
C̅3
O̅4
C̅4
H̅7
H̅6
H̅8
7.3°
C̅U
O̅W
H̅2
H̅1
O2
n
2.823
2.927
O1
m

Fig. 21. Structure of Copper Acetate Monohydrate.

Figure 21 is a diagram showing the structure of copper acetate monohydrate that was determined with the four-circle diffractometer.

The 30-m Small-Angle Neutron Scattering (SANS) Facility

Also located at HB-4 is the 30-m SANS facility, a joint National Science Foundation-Department of Energy-Oak Ridge National Laboratory (NSF-DOE-ORNL) project. The facility, shown in Fig. 22, utilizes pinhole geometry with collimating slits of 0.5- to 3.0-cm diam separated by a distance of 10 m. The detector, with an active area of 64 by 64 cm^2 and resolution element dimensions of 0.5 by 0.5 cm^2, can be positioned at any distance from 1.5 to 18.5 m from the specimen by moving a motor-driven detector carrier along rails in the evacuated flight path. The standard incident wavelength, provided by a bank of pyrolytic graphite crystals, is 4.75 Å; this can be changed to 2.38 Å by substituting graphite for the cold beryllium filter normally in position. The changeover time is less than 5 min, and the procedure permits experiments to be performed with increased flux over a wider range of scattering angles. With 1- by 1-cm slits, the 4.75 Å flux at the sample position is 3.5×10^4 neutrons/cm^2 sec.

This facility is part of the National Center for Small-Angle Scattering Research (NCSASR), sponsored by NSF through an interagency agreement with DOE. Beam time on this instrument is obtained by submitting a proposal to the NCSASR for review by an outside panel of experts who judge the quality of the research proposal. Proposal forms and a general guide to the NCSASR facilities may be obtained from NCSASR Secretary, Solid State Division, Oak Ridge National Laboratory, P.O. Box X, Oak Ridge, Tenn. 37830.

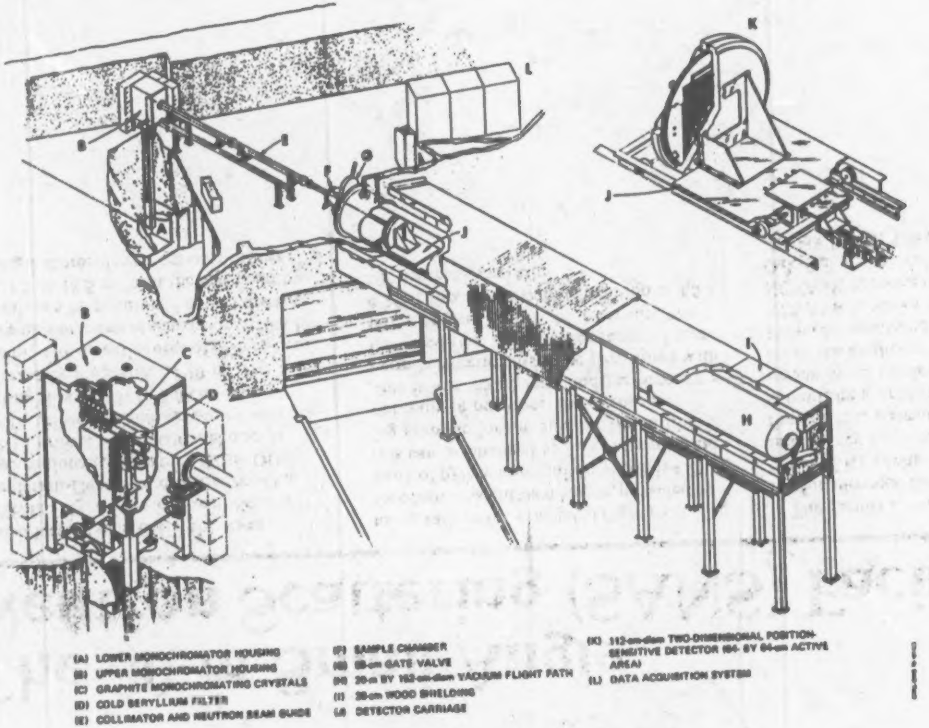

A
B
C
D
E
F
G
H
I
J
K
L
(A) LOWER MONOCHROMATOR HOUSING
(B) UPPER MONOCHROMATOR HOUSING
(C) GRAPHITE MONOCHROMATING CRYSTALS
(D) COLD BERYLLIUM FILTER
(E) COLLIMATOR AND NEUTRON BEAM GUIDE
(F) SAMPLE CHAMBER
(G) 50-cm GATE VALVE
(H) 20-m BY 152-cm-diam VACUUM FLIGHT PATH
(I) 20-cm WOOD SHIELDING
(J) DETECTOR CARRIAGE
(K) 112-cm-diam TWO-DIMENSIONAL POSITION-SENSITIVE DETECTOR (64- BY 64-cm ACTIVE AREA)
(L) DATA ACQUISITION SYSTEM

Fig. 22. 30-m Small-Angle Neutron Scattering Facility.

Data Acquisition System

The major components of the data acquisition system (Fig. 23) for the spectrometers located at HB-1, -1A, -2, and -3 are four PDP 11/23 satellite computers, one for each of these spectrometers, and a fifth host computer, a PDP 11/34. Each satellite computer has 64 K words of memory, two 2.5-M word disks, one Decwriter II, one Tektronix 4006 graphics terminal, and CAMAC interfacing to the experiment. The host computer has 128 K words of memory, four 2.5-M word disks (initially), one high-speed Decwriter III, one DEC VT100 graphics terminal, one Tektronix 4014 graphics terminal, and a Versatec 1200 plotter line printer.

The system software for each satellite and the host is DEC RSX-11M, which allows for multiuser, multitask real-time data acquisition, data analysis and display, and program development; DECNET software is used to provide communication between each satellite computer and the host computer. Each satellite computer is a completely self-contained data acquisition system that provides experimental control and some data analysis and display capabilities. To carry out extensive or complex data reduction, plotting, and analysis, the data can be transferred to the host computer via DECNET. For very extensive data analysis problems, a direct line to the ORNL PDP-10 computer is provided.

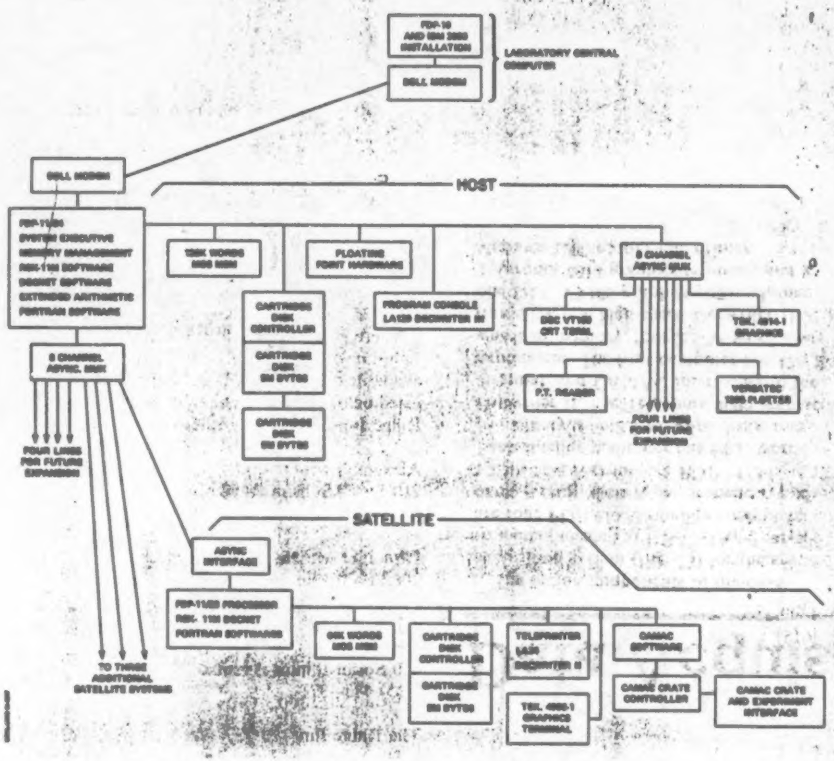

INSTALLATION
LABORATORY CENTRAL COMPUTER
BELL MODEM
BELL MODEM
HOST
SYSTEM EXECUTIVE
MEMORY MANAGEMENT
RSX-11M SOFTWARE
DECNET SOFTWARE
EXTENDED ARITHMETIC
FORTRAN SOFTWARE
8 CHANNEL ASYNC. MUX
FOUR LINES FOR FUTURE EXPANSION
FLOATING POINT HARDWARE
CARTRIDGE DISK CONTROLLER
CARTRIDGE DISK
CARTRIDGE DISK
PROGRAM CONSOLE
8 CHANNEL ASYNC MUX
CRT TERML
P.T. READER
GRAPHICS
VERSATEC
FOUR LINES FOR FUTURE EXPANSION
SATELLITE
ASYNC INTERFACE
FORTRAN SOFTWARE
TO THREE ADDITIONAL SATELLITE SYSTEMS
MOS MEM
CARTRIDGE DISK CONTROLLER
CARTRIDGE DISK
TELEPRINTER
GRAPHICS TERMINAL
CAMAC SOFTWARE
CAMAC CRATE CONTROLLER
CAMAC CRATE AND EXPERIMENT INTERFACE

Fig. 23. Schematic Diagram of the Data Acquisition System.

Auxiliary Equipment

The auxiliary equipment available for controlling sample environment during the neutron experiments includes a variety of cryostats, refrigerators, furnaces, and magnets. For reduced temperatures, there are eight closed-cycle refrigerator units; these are very convenient in the 10 to 300 K range. For lower temperatures, there are three general-purpose liquid-helium cryostats that cover the range 1.2 to 300 K; a ^{3}He cryostat extends this range down to 0.3 K. For elevated temperatures, there are three furnaces and their associated temperature controllers that cover the 300 to 1500 K range.

For problems that require an applied magnetic field, there is a superconducting magnet and a conventional electromagnet. The superconducting magnet has asymmetric split-coil geometry and provides a vertical field of up to 5 T in a 2.5-cm bore. The sample temperature range is 1.2 to 300 K. The electromagnet has tapered pole tips that allow 60° accessibility and an air gap that is continuously variable from 0 to 15 cm. With a 3-cm gap, a field of 2 T is obtained. This magnet is mounted on a cradle that allows 180° rotation about the horizontal axis.

Neutron Wavelength-Energy Relationships

$\lambda(\text{Å}) = 9.044/\sqrt{\epsilon(\text{meV})}$

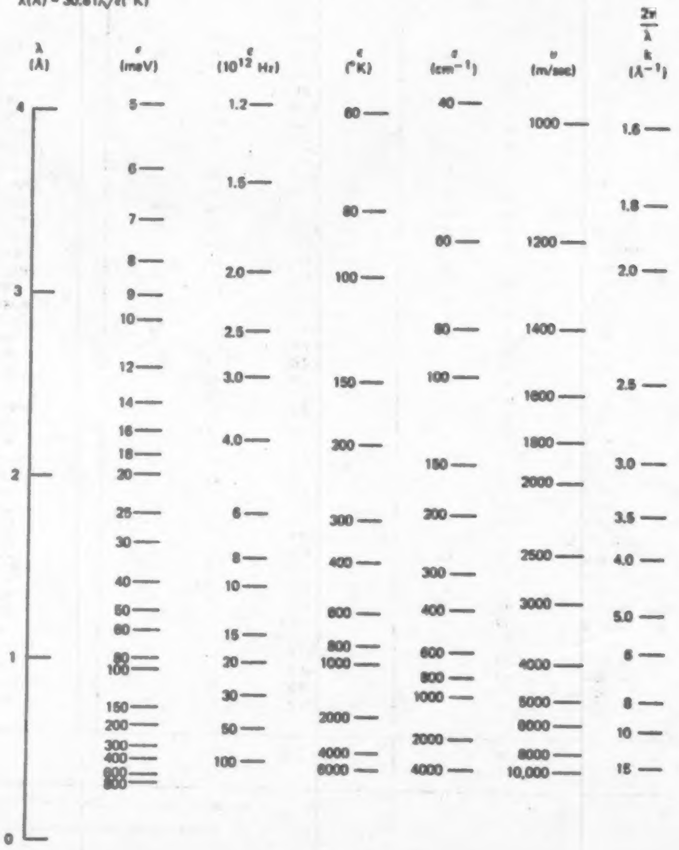
$\lambda(\text{Å}) = 4.447/\sqrt{\epsilon(10^{12}\ \text{Hz})}$

$\lambda(\text{Å}) = 30.81/\sqrt{\epsilon(°\text{K})}$

$\lambda(\text{Å}) = 25.68/\sqrt{\epsilon(\text{cm}^{-1})}$

$\lambda(\text{Å}) = 3956/v(\text{m/sec})$

$\lambda(\text{Å}) = 6.283/k\ (\text{Å}^{-1})$



Coherent Neutron Scattering Amplitudes

(Compiled February, 1972, M.I.T. by C. G. Shull)

Z	Element or isotope	b_{coh}	Z	Element or isotope	b_{coh}	Z	Element or isotope	b_{coh}	Z	Element or isotope	b_{coh}
1	H	−0.3740(3)	23	V	−0.052(3)	47	Ag	0.597(1)		Dy^{161}	1.03
	D	0.6672(7)	24	Cr	0.3532(10)		Ag^{107}	0.83		Dy^{162}	−0.14
	H^{3}	0.47		Cr^{52}	0.490		Ag^{109}	0.43		Dy^{163}	0.50
2	He^{4}	0.30	25	Mn	−0.387(4)	48	Cd	0.37+0.16i		Dy^{164}	4.94
3	Li	−0.214(2)	26	Fe	0.951		Cd^{113}	−1.5+1.2i	67	Ho	0.85
	Li^{6}	0.3+0.025i		Fe^{54}	0.42	49	In	0.39	68	Er	0.800(3)
	Li^{7}	−0.233		Fe^{56}	1.01	50	Sn	0.61	69	Tm	0.720(6)
4	Be	0.774		Fe^{57}	0.23		Sn^{116}	0.58	70	Yb	1.283(6)
5	B	0.534(5)+0.021i	27	Co	0.250		Sn^{117}	0.64	71	Lu	0.73
	B^{11}	0.60	28	Ni	1.03		Sn^{118}	0.58	72	Hf	0.78
6	C	0.6648(3)		Ni^{58}	1.44		Sn^{119}	0.60	73	Ta	0.691(7)
	C^{13}	0.60		Ni^{60}	0.282		Sn^{120}	0.64	74	W	0.477(5)
7	N	0.940		Ni^{61}	0.76		Sn^{122}	0.55		W^{182}	0.88
8	O	0.5803(6)		Ni^{62}	−0.87		Sn^{124}	0.59		W^{183}	0.48
	O^{17}	0.578		Ni^{64}	−0.037	51	Sb	0.5641(13)		W^{184}	0.76
	O^{18}	0.600	29	Cu	0.76	52	Te	0.543(4)		W^{186}	−0.119
9	F	0.5650(11)		Cu^{63}	0.67		Te^{120}	0.52	75	Re	0.92
10	Ne	0.46		Cu^{65}	1.11		Te^{123}	0.57	76	Os	1.07
11	Na	0.362(2)	30	Zn	0.57		Te^{124}	0.55		Os^{188}	0.78
12	Mg	0.532(5)		Zn^{64}	0.56		Te^{125}	0.56		Os^{189}	1.10
13	Al	0.3449(9)		Zn^{66}	0.63	53	I	0.528(2)		Os^{190}	1.14
14	Si	0.4150(1)		Zn^{68}	0.67	54	Xe	0.480		Os^{192}	1.19
15	P	0.51	31	Ga	0.72	55	Cs	0.541(3)	77	Ir	1.06
16	S	0.2847(1)	32	Ge	0.8186(3)	56	Ba	0.512(5)	78	Pt	0.95
17	Cl	0.9580(2)	33	As	0.64	57	La	0.83	79	Au	0.76
	Cl^{35}	1.18	34	Se	0.797(2)	58	Ce	0.482(3)	80	Hg	1.266(2)
	Cl^{37}	0.26	35	Br	0.679(1)		Ce^{140}	0.47	81	Tl	0.890(2)
18	A	0.20	36	Kr	0.74		Ce^{142}	0.45	82	Pb	0.9404(4)
	A^{36}	2.43	37	Rb	0.708(2)	59	Pr	0.44	83	Bi	0.8523(2)
19	K	0.370(2)		Rb^{85}	0.83	60	Nd	0.72	90	Th	1.033(3)
	K^{39}	0.37	38	Sr	0.700(8)		Nd^{142}	0.77	92	U	0.853(4)
20	Ca	0.466(3)	39	Y	0.79		Nd^{144}	0.28		U^{235}	0.98
	Ca^{40}	0.49	40	Zr	0.714(3)		Nd^{146}	0.87		U^{238}	0.85
	Ca^{44}	0.18	41	Nb	0.711(4)	62	Sm^{152}	−0.5	93	Np	1.055
21	Sc	1.18	42	Mo	0.688(5)		Sm^{154}	0.8	94	Pu^{239}	0.75
22	Ti	−0.335(3)	43	Tc^{99}	0.68	63	Eu	0.55		Pu^{240}	0.35
	Ti^{46}	0.48	44	Ru	0.726(4)	64	Gd	1.5		Pu^{242}	0.81
	Ti^{47}	0.33	45	Rh	0.584(4)	65	Tb	0.76			
	Ti^{48}	−0.58	46	Pd	0.60	66	Dy	1.69			
	Ti^{49}	0.08					Dy^{160}	0.67			
	Ti^{50}	0.55									

Bragg Angles $2\theta_m$, Wavelengths, and Energies for Commonly Used Monochromators

2 THETA (DEG)	BERYLLIUM(002) D = 1.792 Å		GRAPHITE(002) D = 3.348 Å		GERMANIUM(111) D = 3.266 Å		IRON-57(110) D = 2.020 Å	
	E(meV)	λ(Å)	E(meV)	λ(Å)	E(meV)	λ(Å)	E(meV)	λ(Å)
10	838.74	0.3123	240.18	0.5836	252.35	0.5693	659.66	0.3521
11	693.54	0.3434	198.60	0.6418	208.67	0.6261	545.46	0.3873
12	583.11	0.3745	166.98	0.6999	175.44	0.6828	458.61	0.4223
13	497.16	0.4056	142.37	0.7580	149.58	0.7395	391.02	0.4574
14	428.97	0.4367	122.84	0.8160	129.06	0.7961	337.38	0.4924
15	373.96	0.4677	107.09	0.8740	112.51	0.8527	294.11	0.5274
16	328.93	0.4987	94.19	0.9319	98.97	0.9092	258.70	0.5623
17	291.62	0.5296	83.51	0.9897	87.74	0.9656	229.35	0.5972
18	260.35	0.5605	74.55	1.0475	78.33	1.0219	204.76	0.6321
19	233.88	0.5914	66.97	1.1052	70.37	1.0782	183.95	0.6669
20	211.29	0.6222	60.50	1.1627	63.57	1.1344	166.18	0.7016
21	191.85	0.6530	54.94	1.2202	57.72	1.1905	150.88	0.7363
22	174.99	0.6837	50.11	1.2777	52.65	1.2465	137.63	0.7709
23	160.29	0.7144	45.90	1.3350	48.23	1.3024	126.07	0.8055
24	147.39	0.7450	42.21	1.3922	44.34	1.3582	115.92	0.8400
25	136.00	0.7755	38.95	1.4493	40.92	1.4139	106.96	0.8745
26	125.90	0.8060	36.05	1.5063	37.88	1.4695	99.02	0.9089
27	116.91	0.8365	33.48	1.5632	35.17	1.5250	91.95	0.9432
28	108.86	0.8669	31.17	1.6199	32.75	1.5804	85.62	0.9775
29	101.63	0.8972	29.10	1.6765	30.58	1.6356	79.93	1.0116
30	95.11	0.9274	27.24	1.7331	28.62	1.6907	74.80	1.0457
31	89.21	0.9576	25.55	1.7894	26.84	1.7457	70.16	1.0797
32	83.86	0.9877	24.01	1.8457	25.23	1.8006	65.95	1.1137
33	78.98	1.0177	22.62	1.9018	23.76	1.8553	62.12	1.1475
34	74.53	1.0476	21.34	1.9577	22.42	1.9099	58.62	1.1813
35	70.46	1.0775	20.18	2.0135	21.20	1.9644	55.41	1.2150
36	66.72	1.1073	19.11	2.0692	20.07	2.0187	52.47	1.2486
37	63.28	1.1370	18.12	2.1247	19.04	2.0728	49.77	1.2820
38	60.11	1.1666	17.21	2.1800	18.08	2.1268	47.27	1.3154
39	57.18	1.1961	16.37	2.2352	17.20	2.1806	44.97	1.3487
40	54.46	1.2255	15.60	2.2902	16.39	2.2343	42.84	1.3819
41	51.95	1.2549	14.88	2.3450	15.63	2.2877	40.86	1.4150
42	49.61	1.2841	14.21	2.3996	14.93	2.3411	39.02	1.4479
43	47.43	1.3132	13.58	2.4541	14.27	2.3942	37.30	1.4808
44	45.40	1.3423	13.00	2.5084	13.66	2.4471	35.71	1.5136
45	43.50	1.3712	12.46	2.5624	13.09	2.4999	34.22	1.5462
46	41.73	1.4001	11.95	2.6163	12.56	2.5525	32.82	1.5787
47	40.07	1.4288	11.47	2.6700	12.06	2.6048	31.51	1.6111
48	38.51	1.4574	11.03	2.7235	11.59	2.6570	30.29	1.6434
49	37.05	1.4859	10.61	2.7768	11.15	2.7090	29.14	1.6755

2 THETA (DEG)	BERYLLIUM(002) D = 1.792 Å		GRAPHITE(002) D = 3.348 Å		GERMANIUM(111) D = 3.266 Å		IRON-57(110) D = 2.020 Å	
	E(meV)	λ(Å)	E(meV)	λ(Å)	E(meV)	λ(Å)	E(meV)	λ(Å)
50	35.67	1.5143	10.21	2.8299	10.73	2.7608	28.06	1.7075
51	34.38	1.5426	9.84	2.8827	10.34	2.8123	27.04	1.7394
52	33.15	1.5708	9.49	2.9353	9.97	2.8637	26.08	1.7712
53	32.00	1.5988	9.16	2.9877	9.63	2.9148	25.17	1.8028
54	30.91	1.6267	8.85	3.0399	9.30	2.9657	24.31	1.8343
55	29.88	1.6545	8.56	3.0919	8.99	3.0164	23.50	1.8656
56	28.91	1.6822	8.28	3.1436	8.70	3.0668	22.73	1.8969
57	27.98	1.7098	8.01	3.1951	8.42	3.1171	22.01	1.9279
58	27.11	1.7372	7.76	3.2463	8.16	3.1670	21.32	1.9588
59	26.27	1.7645	7.52	3.2973	7.91	3.2168	20.66	1.9896
60	25.48	1.7916	7.30	3.3480	7.67	3.2663	20.04	2.0202
61	24.73	1.8186	7.08	3.3985	7.44	3.3155	19.45	2.0507
62	24.02	1.8455	6.88	3.4487	7.23	3.3645	18.89	2.0810
63	23.34	1.8722	6.68	3.4987	7.02	3.4132	18.35	2.1111
64	22.69	1.8988	6.50	3.5483	6.83	3.4617	17.84	2.1411
65	22.07	1.9253	6.32	3.5978	6.64	3.5099	17.36	2.1709
66	21.48	1.9516	6.15	3.6469	6.46	3.5579	16.89	2.2006
67	20.91	1.9777	5.99	3.6958	6.29	3.6056	16.45	2.2300
68	20.37	2.0037	5.83	3.7444	6.13	3.6530	16.02	2.2594
69	19.86	2.0295	5.69	3.7927	5.98	3.7001	15.62	2.2885
70	19.37	2.0552	5.55	3.8407	5.83	3.7469	15.23	2.3175
71	18.89	2.0808	5.41	3.8884	5.68	3.7935	14.86	2.3463
72	18.44	2.1062	5.28	3.9358	5.55	3.8397	14.50	2.3749
73	18.01	2.1314	5.16	3.9829	5.42	3.8857	14.16	2.4033
74	17.59	2.1564	5.04	4.0298	5.29	3.9314	13.84	2.4316
75	17.19	2.1813	4.92	4.0763	5.17	3.9768	13.52	2.4596
77	16.44	2.2306	4.71	4.1684	4.95	4.0666	12.93	2.5152
78	16.09	2.2550	4.61	4.2139	4.84	4.1111	12.65	2.5427
79	15.75	2.2792	4.51	4.2592	4.74	4.1552	12.38	2.5700
80	15.42	2.3032	4.42	4.3041	4.64	4.1990	12.13	2.5971
81	15.11	2.3271	4.33	4.3487	4.54	4.2425	11.88	2.6240
82	14.80	2.3508	4.24	4.3930	4.45	4.2857	11.64	2.6507
83	14.51	2.3743	4.16	4.4369	4.37	4.3286	11.41	2.6773
84	14.23	2.3976	4.07	4.4805	4.28	4.3711	11.19	2.7036
85	13.96	2.4208	4.00	4.5238	4.20	4.4133	10.98	2.7297
86	13.70	2.4437	3.92	4.5667	4.12	4.4552	10.77	2.7555
87	13.45	2.4665	3.85	4.6092	4.05	4.4967	10.58	2.7812
88	13.20	2.4891	3.78	4.6514	3.97	4.5379	10.38	2.8067
89	12.97	2.5115	3.71	4.6933	3.90	4.5787	10.20	2.8320
90	12.74	2.5337	3.65	4.7348	3.83	4.6192	10.02	2.8570

8.4 National Center for Small-Angle Scattering Research

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

   Answer: This facility is supported by NSF. Small-angle scattering of neutrons or x-rays is a technique for studying structures of matter on a global scale, that is, of dimensions from a few tens to a few thousands of angstroms. Small-angle neutron scattering is particularly useful in substances that contain hydrogen because the scattering length density can be modified by substituting deuterium for hydrogen, the so-called contrast variation technique. Diverse studies have been carried out in areas such as polymer science, metallurgy and materials science, physical chemistry, magnetism, superconductivity, and biology.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

   Answer: The NCSASR provides experimental facilities to the American scientific community for small-angle neutron scattering (SANS) research that are unequaled in the United States from the aspect of resolution, ease of operation, user-friendly software, and staff expertise in the major areas of application. The SANS instrument is a national user-oriented facility, time on which is assigned solely on the basis of scientific merit. As such, it is unique in the United States.

   The 10-m SAXS camera, for which one-third time is allocated to the NCSASR, is a unique instrument in the world at the present time. It is equipped with a position-sensitive area detector and a very fast data acquisition system. An elegant sample deformation device has recently been developed for use with it. A new 12 kW generator will greatly expand the capabilities of this instrument for time-slicing experiments.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

   Answer: The NCSASR provides the following experimental facilities to the American scientific community on a user-oriented basis.

   1. Full time use of the ORNL-NSF-DOE 30-m small-angle neutron scattering (SANS) instrument.

   2. Part-time use of DOE constructed instruments:

      a. 10-m SANS instrument at the ORR.
      b. Double-perfect crystal SANS (for extremely high-resolution) at the HFIR.
      c. 10-m SAXS camera with position-sensitive area detector based on rotating anode source.
      d. Kratky SAXS camera with position-sensitive linear detector.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer: The research accomplished with the facilities of the NCSASR consists of that proposed by the user community and that of the Center's staff. Each member of the staff is encouraged to, and indeed, expected to, carry out an active research program of his own. All research, internal and external, is subject to review by the Program Committee. Work has been done in the area of polymer science -- particularly the study of polymer blends (alloys). Many experiments have been done in the study of latexes and micelles, of critical scattering in magnetic materials, of phase transformations in alloys, of stress induced cavitation in metals, alloys, and ceramics, of the structure of superconducting materials, of dynamic deformation of polymers and composites, and of the structure of biological systems. It is expected that work in dynamics of polymer systems and of the kinetics of gel and microemulsion formation will be active areas in the future.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: The 30-m ORNL-NSF-DOE small-angle neutron scattering facility was constructed under an interagency agreement effective January 1, 1978. It became operational, in a routine user-oriented mode in October 1980.

Since then i) a biological preparations laboratory has been built adjacent to the instrument and basic equipment installed, ii) an improved data acquisition system installed, iii) automatic sample changers for solid and liquid samples have been built. With the shutdown of the reactor (HFIR) in the latter part of 1983 for reflector replacement, horizontal and vertical neutron beam guide sections were and are being installed to add intensity and flexibility to the operation of the instrument.

The x-ray instrument was equipped with a sophisticated data acquisition system for use with a newly constructed sample-deformation device. A new 12 kW rotating anode source will permit elegant time-slicing experiments to be performed.

The 10-m instrument at the ORR has been completely rebuilt with a 64 x 64 cm^2 position-sensitive area detector. It will be used in part for ORNL programmatic research and in part to complement the use of the 30-m machine.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer:

	B/A (Dollars in Thousands)				
Item	CY 1981	CY 1982	CY 1983	CY 1984	CY 1985
Operations - NSF	$ 463	$ 486	$ 472	$ 466	$ 625
In-House Research	188	195	181	179	242
BES - Materials Sciences	100	100	90	90	100
National Science Foundation	88	95	91	89	142
Out-of-House Research*	1,200	1,200	800	800	1,200
Other Operating Expense	0	0	0	0	0
Capital Equipment - NSF	0	0	60	100	26
AIP	0	0	0	0	0
General Plant Projects	0	0	0	0	0
In-House Energy Management	0	0	0	0	0
Other Construction	0	124	0	0	0
TOTAL	$1,851	$2,005	$1,513	$1,545	$2,093

* This research is funded by sources in NSF, DOD, Other DOE, Industry, etc. and obtained by the institutions doing the research and is usually not known by ORNL.

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer: All direct funding for the NCSASR has been and is expected to be provided by the National Science Foundation. Contracts with several industrial organizations to carry out proprietary research on a cost recovery basis have been concluded. Some two thousand dollars have been paid into the Center from this source. It is expected that modest sums will continue to be realized from proprietary research.

All indirect funding (e.g. travel, living expenses, sample preparation, etc.) for users is furnished by the users' institutions or by grants from federal agencies to the users.

8. **For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.**

Answer: Staffing Levels

1981	1982	(FTE) 1983	1984	1985
4	4.5	4.5	4.5	6.0

This is primarily an NSF supported facility. For example, NSF supports 3.5 FTE in FY 1984 and the Division of Materials Sciences, DOE supports 1.0.

9. **What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?**

Answer: The 30-m SANS facility is fully utilized. The HFIR operates 93% of the year. Full usage of the instrument means that the facility is in use by an experimenter or by a staff member for machine physics or development at all times that the reactor is operating. Experiments are generally scheduled three months in advance and all time is fully booked.

10. **For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?**

Answer: Experiments started and completed

1981	1982	1983*	1984*	1985
80	100	80	80 est	150 est

* The SANS facility was not operating for the last quarter of CY 1983 and the first quarter of CY 1984 due to the replacement of the reflector in the reactor. The number of "experiments" has been interpreted as the number of proposals. Nearly all proposals involve several different materials and external sample conditions. Consequently, in a strict sense, each number listed above could be at least 5 times higher.

11. **What is this facility's user policy?**

Answer: The NCSASR is a National user-oriented facility. All beam time on the 30-m instrument and about 1/3 of the time on the 10-m SANS and 10-m SAXS machines is assigned to users, external and internal.

12. **For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?**

Answer: Contracts for the accomplishment of proprietary research have been negotiated with du Pont, Firestone, and Eastman Kodak. Costs are assessed on a full-cost recovery basis. About $2000.00 has been received from this source. Modest use of this option is anticipated for the balance of 1984 and for 1985.

13. **What is the mechanism by which specific research proposals for experiments at the facility are considered?**

Answer: Research proposals for use of the facilities of the NCSASR are evaluated on the basis of scientific merit, by an external committee of experts. Time is assigned by NCSASR staff if favorable referees' reports have been received. The time lapse is usually not more than three months between receipt of the proposal and assignment of beam time.

14. How many research proposals have been submitted over the past five years, and how many of these have been approved?

Answer: From October 1980 until March 1984, 251 proposals have been received. Of these 95% have eventually been accepted. In many cases, following a referee's recommendation, a proposal has been rewritten and resubmitted.

15. How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?

Answer: Since October 1980, 110 university personnel have used the NCSASR facilities. Most of these people have used the facilities several times during this period.

16. How many industrial researchers have utilized the facility over the past five years?

Answer: Since October 1980, 31 industrial users have used the NCSASR facilities. Most of these people have used the facilities several times during this period.

17. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer: Since October 1980, 20 foreign investigators have used the NCSASR facilities. Some of these investigators have used the facilities several times during this period.

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: Since October 1980, 39 investigators from government agencies have used the NCSASR facilities. Many of these investigators have used the facilities several times during this period.

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: A study has been initiated to modify significantly the HFIR or to build a new reactor at Oak Ridge. Cold sources and guide halls are envisaged. The SANS facility would be moved to a cold guide, and a second one constructed. Meanwhile, efforts will be continued to improve background and flux on the sample and to improve instrument stability. Time-slicing capability on samples in nonequilibrium states will be developed.

20. Please provide a copy of the facility's latest annual report.

Answer: Excerpts from the facility's latest annual report are attached.

NATIONAL CENTER FOR SMALL-ANGLE
SCATTERING RESEARCH

Report of Activities

October 1, 1981 - September 30, 1982

NATIONAL CENTER FOR SMALL-ANGLE SCATTERING RESEARCH

October 1982

The activities of the National Center for Small-Angle Scattering Research for the period October 1, 1981 - September 30, 1982, are summarized. We report on the status of the 30-m SANS facility, the 10-m SAXS camera, the administration, use of the Center's facilities, and the staff, and we include a short discussion of some of the short-term problems facing the Center.

30-M SANS Facility

During the period of this report, the 30-m SANS facility operated routinely, with little unscheduled downtime. In view of the greater operational reliability of the system, less time has been devoted to machine physics and repairs (~1 day per week) with users scheduled, generally, for the remaining six days.

The repairs on the first detector have gone much more slowly than expected. A gas purification and handling system has been built and preliminary tests on the new low gamma-sensitive fill gas were very encouraging, suggesting a substantial reduction in the overall gamma-ray background counting rate. During high-voltage run up of the detector a wire broke on one of the cathode planes and it was necessary to open the system and do some restringing. It is now expected that the detector with the new fill gas will be ready for installation at the end of November 1982.

The construction of the computer enclosure and the biological preparation laboratory is proceeding but also more slowly than expected. A temporary air conditioned tent is being constructed around the computer and the terminals, so that the instrument can be used during the worst of the dust producing construction activities. Construction is now expected to be completed at the end of January 1983.

Many of the users have been able to work more efficiently during this report period as a result of the successful operation of an automatic, computer-controlled sample changer for solid specimens and for liquids in sealed cells. Software has been written to permit the first stages of data reduction to be done automatically as well. At present a user can set up as many as eight samples for an over-night run and return in the morning to find the data corrected for background and detector sensitivity variation, radially averaged, and stored on disk in one dimensional files ready for further analysis.

The design for an automatic sample changer for cells containing liquid samples, at controlled temperatures ranging from -10°C to +130°C, with provision for providing a moisture-free atmosphere (to prevent condensation) has been completed. Construction will be started as funding is assured. This will be particularly useful for users in the biological, chemical, and polymer areas.

Improvements in software for data analyses are being made, usually as a result of the needs of specific experiments. A very general program for the analysis of data on micellar and similar systems has been developed, principally by R. Triolo, a user, and H. R. Child. This program draws on software provided by John Hayter of the I.L.L. and it enables each user to fit his data to his own model. For polymer applications programs are now available which enable the user to fit a wide range of the scattering curve to the Debye function for a random coil, rather than making use of the Guinier or Zimm approximations over a limited angular range, for purposes of extracting particle dimensions and molecular weights.

Funding has been provided for the horizontal guide sections and design for this improvement to the system is underway.

10-M SAXS Camera

The 10-m SAXS facility has operated, during the last year, with relatively little downtime. Several months have been dedicated to studies of polymer deformation in which the 256 K Mostek memory has been used to store time-sliced data. The software development for the operation of dynamic deformation device and the analysis of dynamic data is complete and ready for routine experimentation. The device may now be said to be operational, and the first publications are being submitted to journals and symposia.

A specially designed sample holder with a temperature controller and fast quenching arrangement has been made available through collaboration with Professors J. H. Magill and J. M. Schultz for the kinetic and crystallization study. The high temperature limit is tentatively set at 300°C. Many of the improvements in data handling and presentation developed for the 30-m SANS instrument have been incorporated in the software package for the SAXS camera. In particular, background corrections for weakly scattering samples can now be applied correctly in floating point format, thus avoiding the round off errors associated with the previous programs.

Staff

The staff of the Center has stabilized during this report period. Personnel for the maintenance and improvement of the SAS instruments, including the dynamic deformation device, are hired on an as-needed basis from the Instruments and Controls Division of the Laboratory. The software maintenance and development for all SAS instrumentation is under the supervision of H. R. Child with Linda Maddox of the ORNL Computer Sciences Division.

Dr. S. Spooner joined the staff of the Solid State Division and the NCSASR on December 21, 1981. His principal responsibilities are the execution of the materials and metallurgy programs of the Solid State Division. He has in addition provided assistance to and interaction with external users of the NCSASR facilities whose interests are in the metallurgy area.

Dr. V. Ramakrishnan has been a member of the NCSASR staff since February 9, 1982. He is responsible for interactions with users with problems in areas of biology, and for developing a biologically oriented user community.

Professor Toshio Kitao, Kyoto University of Industrial Arts and Textile Science, has worked closely with J. S. Lin, on a half-time basis, in the x-ray laboratory since December 1, 1981. He has supervised the work of graduate students in the Department of Polymer Engineering at the University of Tennessee, as well as having carried out a research program on the mechanical properties of laminated polymers and fibers He will return to Japan on or about December 1, 1982.

Admininstration

With approval and agreement of the members of the Advisory Committee, the retiring members in 1981, C. Wert and H. Brumberger, were not replaced, thus reducing the Committee size to one of four members. A meeting of this Committee is scheduled for November 1, 1982, at the Oak Ridge National Laboratory.

A contract for the performance of proprietary reseach has been executed with the Eastman Kodak Company.

The second NCSASR Users' Group meeting, organized by the users' group Executive Committee (John King, Jerry Schultz, Robert Ullman, Julia Weertman, Charles Berney, Ernest Epperson, Charles Han, and Hyuk Yu) was held at the Oak Ridge National Laboratory November 16 and 17, 1981. Some 40 scientists attended the meeting. A copy of the program appears as Appendix A, and a copy of the resolutions adopted by the participants is given in Appendix B.

The cooperation of the administration of Oak Ridge Associated Universities (ORAU) has permitted us to continue to provide users the use of an automobile at a nominal daily charge ($5.00). The lodging difficulties we had anticipated during the 1982 World's Fair in Knoxville were solved by warning our users to book as early as possible, and by use of some rooms booked in local motels by the UCC-ND Purchasing Division. No experiments had to be canceled due to a lack of accommodation, although the price of hotel rooms was appreciably higher than normal. For users needing modestly priced accommodation we were generally able to provide a bed in an apartment rented by the Ames Laboratory (Iowa State University) at a nominal charge. We will try to continue to furnish this service after the Fair closes on October 31, 1982. We are grateful to the Ames Laboratory staff for their cooperation.

The guides to the use of the SAS facilities are now reaching what we hope are their final versions.

Use of the Facilities

In this report period some 42 proposals have been received. This number does not fairly represent the use of the facilities in as much as many scientists have had several sessions of instrument time for one proposal. In many cases these repetitions are legitimate, in accordance with our announced policy for granting beam time in more than one time period. In others, the work has drifted sufficiently far from the purpose originally stated that a new proposal is warranted. We propose to evaluate all outstanding proposals, and close them out where the facts indicate.

We list the new proposals, making a total of 180, in Appendix C. As in past years, we attach Appendix D, the Research Reports submitted by the users during the reporting period.

As a natural consequence of the maturity of the installations and the growing expertise of the users, there is an increasing number of publications resulting from work done under the auspices of the NCSASR. The publications of this report period are listed in Appendix E.

Short Term Problems

The High Flux Isotope Reactor is a light water-cooled, light water-moderated, beryllium-reflected reactor. Approximately every nine years, according to calculation (and experience) it is necessary to replace the beryllium reflector in order to avoid problems associated with flaking and cracking due to irradiation damage.

The second such reflector replacement is scheduled to begin on October 1, 1983. If this replacement proceeds on the same schedule as the first one, the reactor itself will be down three months. However, the instrumentation will be inoperative for somewhat longer periods depending upon the beam tube with which it is associated. The 30-m SANS facility, associated with HB-4 will be down approximately 6 months because HB-4 will be the first of the beam ports to be dismantled, and the last to be replaced.

A number of improvements and repairs will be made (new graphite, improved motor drivers and controls) to the 30-m SANS facility, during this time, that will result in a much more powerful instrument. In the interim, however, we wish to provide our users with the possibility of carrying out some, at least, of their experiments.

To that end we propose, starting immediately, to reactivate the SANS facility at the ORR. During the past year this facility has been extremely useful to the staff and users as a computational center, but because the 20 x 20 cm^2 detector originally used was no longer serviceable, it has not been used as an experimental facility.

With the backup 64 x 64 cm^2 detector and the new fill gas, we propose to build a fixed distance instrument that will satisfy the needs of users with moderately and strongly scattering specimens. We will need to construct shielding for the detector and a new shielded flight-path from sample to detector. In addition, we plan to use the monochromator system formerly used at HB-3 of the ORR on a long term loan. We believe that an improvement in flux of a factor of the order of 4-5 can be obtained.

This concept is not new. It was proposed as a joint project between NSF and DOE in the three-year budget proposal beginning January 1, 1981. We have requested the sum of $33,000 from the NSF in the CY 1983 proposal for funds to cover one-third the cost of this installation. The remaining two-thirds will be requested from ORNL and DOE sources. It is our intention to use the improved ORR machine after the reflector replacement is complete, to accommodate DOE and NSF users for those problems that can be done there, and thus to absorb some of the over subscription of the 30-m machine that is beginning, even now, to develop.

APPENDIX A

Program for the Second NCSASR Users' Group Meeting.

SECOND NCSASR USERS' GROUP MEETING
November 16 & 17, 1981
East Auditorium, Oak Ridge National Laboratory

PROGRAM

November 16, 1981

8:00 A.M.	Bus leaves Holiday Inn-Oak Ridge	
8:15 - 8:45	Late Registration at East Auditorium, ORNL	
8:50	Calls to Order	Hyuk Yu, Chairman, Exec. Comm. Users' Group, University of Wisconsin
8:55	Greetings	Alexander Zucker, Assoc. Director, ORNL
9:05 - 9:35	Overview & Summary Report of NCSASR	W. C. Koehler, Director, NCSASR
9:35 - 9:55	NSF Support of NCSASR	W. Oosterhuis, DMR, NSF
9:55 - 10:10	ORAU Support of NCSASR	W. E. Felling, Oak Ridge Associated Universities
10:10 - 10:40	COFFEE BREAK	

Chair: J. H. Schultz - University of Delaware

10:40 - 11:10	Status Report on SANS Facilities	G. D. Wignall, NCSASR
11:10 - 11:20	Question and Answer	
11:20 - 11:50	Status Report on SAXS Facilities	J. S. Lin, NCSASR
11:50 - 12:00	Question and Answer	
12:00 - 12:30	Status Report on Softwares	H. R. Child, NCSASR
12:30 - 12:40	Question and Answer	
12:40 - 2:00	LUNCH	

Chair: J. E. Epperson - Argonne National Laboratory

2:00 - 2:30	SANS Studies of Synthetic Polymers	R. S. Stein, University of Massachusetts
2:30 - 3:00	SANS Studies of a Biological Sample	G. J. Bunick and E. C. Uberbacher, ORNL
3:00 - 3:30	SANS Studies of Metals	J. R. Weertman, Northwestern University
3:30 - 4:00	COFFEE BREAK	
4:00 - 4:30	SAXS Studies of Synthetic Polymers	J. F. Fellers, University of Tennessee
4:30 - 5:00	SAXS Studies of Metals	J. E. Epperson, ANL
5:30	Bus leaves ORNL	
6:00 - 7:30	Reception at Oak Ridge Associated Universities	

NO GROUP DINNER IS PLANNED

November 17, 1981

8:00 A.M.	Bus leaves Holiday Inn-Oak Ridge	
Chair:	Robert Ullman, Ford Motor Company	
8:30 - 8:40	Opening Remarks	
8:40 - 9:10	Recent experience at the Center by an industrial scientist	J. M. O'Reilly, Eastman Kodak Company
9:10 - 9:40	Recent experience by a graduate student	F. S. Bates, Dept. of Chem. Eng'n, M.I.T.
9:40 - 10:10	An experienced user's view of the Center operation	J. M. Schultz, University of Delaware
10:10 - 10:40	The Center staff experience with new users	Center Staff
10:40 - 11:10	COFFEE BREAK	
Chair:	J. S. King, University of Michigan	
11:10 - 11:30	Summary of Recent Questionnaires	
11:30 - 12:30	Round Table Discussion -nature of user oriented national center -potential and constraints of NCSASR -users' desires for the staff responsiveness -technical and non-technical preparations -others	Discussants: Koehler, O'Reilly, Bates, Schultz, Weertman, Ullman, Stein, Schaefer, Oosterhuis, Epperson
12:30 - 2:00	LUNCH	
Chair:	J. R. Weertman - Northwestern University	
2:00 - 2:30	Remarks by Review Committee representative	D. W. Schaefer, Sandia Laboratories
2:30 - 2:40	Question and Answer	
2:40 - 3:00	Summary Remarks	W. C. Koehler
Chair:	Hyuk Yu	
3:00 - 4:00	Business Session of User's Group 1. Election of 4 members of Exec. Comm. 2. Formulation of Recommendations	
4:00	ADJOURN	
4:20	Bus leaves ORNL	

APPENDIX B

Draft Resolution adopted at the NCSASR Users' Meeting November 1981, at ORNL.

Draft Resolution

1. The Users' Group expresses it commendation and appreciation to the staff of NCSASR for their dedicated efforts in constructing, maintaining, and improving the neutron and X-ray instruments that make the NCSASR a unique resource for American science.

2. The Users' Group supports a high priority effort to secure funds to maintain the operation of the 10-meter SAXS instrument, and to insure its accessibility outside the DOE community. This instrument is unique and highly productive in its own right. Furthermore, X-ray and neutron small-angle scattering are essentially complementary techniques; hence, the loss of the 10-meter facility would seriously impair the effectiveness of the Center.

3. Travel expenses for the users are an essential part of the smooth and effective operation of NCSASR. ORAU in the person of Dr. William Felling has helped pursue this goal for two years. The Users' Group expresses its gratitude for his effort on behalf of the user community.

4. The Users' Group will sponsor a national small-angle scattering meeting in the vicinity of Oak Ridge in about two years, with the intention of providing a showcase for the scientific results now emerging from NCSASR and other similiar facilities.

APPENDIX C

List of proposal, by category, received in the period October 1, 1981 - September 30, 1982. (The numbers carry on in sequence from the 1981 report.)

PROPOSALS

Biology

14. SAXS studies of fibrin films, Dr. John D. Ferry - University of Wisconsin, Madison, WI 53706

15. Small-angle scattering study of nucleosome unfolding, Dr. Gerard J. Bunick - Oak Ridge National Laboratory, Oak Ridge, TN 37830

16. SANS study of the cro repressor protein, Dr. Y. Takeda - University of Maryland, Catonsville, MD 21228

17. Small-angle neutron scattering study of F1-ATPase from the thermophilic bacterium PS3, Dr. Y. Kagawa - Minamichikawachi-Machi, Japan.

18. Contrast variation study of deuterated 30S ribosomes from E. Coli, Dr. P. B. Moore - Yale University, New Haven, CT 06520

PROPOSALS

Materials and Chemistry

48. Intercomparison of SANS instruments, Dr. J. Schelten - IFF, Julich W. Germany

49. Particle scattering function of coal and soluble coal derivatives, Dr. H. P. Hombach - Institut fur Kohlenforschung, W. Germany

50. Effect of nitric acid treatment on porosity of activated charcoals, Dr. J. S. Johnson, Jr. - Oak Ridge National Laboratory, Oak Ridge, TN 37830

51. Complex formation in aqueous zinc chloride solutions, Dr. A. H. Narten - Oak Ridge National Laboratory, Oak Ridge, TN 37830

52. Characterization of heat treated and neutron irradiated titanium-modified 316 stainless steels (austenitic), Dr. Stephen Spooner - Oak Ridge National Laboratory, Oak Ridge, TN 37830

53. Investigation of microstructures in ferritic steels. A unirradiated, Dr. Phillip Maziacz - Oak Ridge National Laboratory, Oak Ridge, TN 37830

54. Determination of particle size distribution in Al-Li alloys, Dr. Stephen Spooner - Oak Ridge National Laboratory, Oak Ridge, TN 37830

55. Structure of ion-implanted cooper single crystals: preliminary proposal, Dr. Stephen Spooner - Oak Ridge National Laboratory, Oak Ridge, TN 37830

56. SANS investigations of critical phenomena in microemulsions, Ms. L. J. Magid - University of Tennessee, Knoxville, TN 37916

57. Preliminary investigaton: Nickel precipitates in MgO, Dr. Stephen Spooner - Oak Ridge National Laboratory, Oak Ridge, TN 37830

58. Structure of ionic micelles, Dr. R.R.M. Jones - Wake Forest University, Winston-Salem, NC 27109

59. Void formation in compression creep SiC samples, Dr. James Bentley - Oak Ridge National Laboratory, Oak Ridge, TN 37830

60. Ferrocene distribution in micelles, Dr. R. Triolo, University of Palermo, Palermo, Italy

61. Neutron and x-ray scattering studies of ferrofluid particles, Dr. Anthony C. Nunes - University of Rhode Island, Kingston, RI 02881

62. Small angle x-ray scattering studies of annealed amorphous alloys, Dr. C. C. Koch - Oak Ridge National Laboratory, Oak Ridge, TN 37830

PROPOSALS

Polymer Science

79. Coalescence in heterogeneous polymer blends, Dr. C. M. Roland - Firestone Tire & Rubber Company, Akron, OH 44317

80. SAXS and SANS studies of block copolymers, Dr. Jeff Koberstein - Princeton University, Princeton, NJ 08544

81. SAXS study of defect structures in wet spun biaxially oriented (p-phenylene terephthalamide) films, Dr. J. F. Fellers - University of Tennessee, Knoxville, TN 37916

82. Radial compositional gradients in copolymer latices, Dr. J. M. O'Reilly - Eastman Kodak Company, Rochester, NY 14650

83. Gelatin solutions and gels, Dr. J. M. O'Reilly - Eastman Kodak Company, Rochester, NY 14650

84. Changes in Static Conformation of a single polystyrene long chain in a host of short polystyrene chains. Part I: Limit of the ideal character of the long chain, Prof. J. S. King - University of Michigan, Ann Arbor, MI 48109

85. Polystyrene chain conformation in good solvents: Part I - Reliability of the high concentration doping method, Prof. J. S. King - University of Michigan, Ann Arbor, MI 48109

86. Neutron scattering from latices prepared by seeded emulsion polymerization, Dr. R. A. Gelman - Hercules Incorporated, Wilmington, DE 19899

87. Compatability of polyethylene blends, Dr. F. C. Stehling - Exxon Chemical Company, Baytown, TX 77520

88. Carbon filled polymers, Dr. S. Morris - Raychem Corporation, Menlo Park, CA 94025

89. Transesterification in poly(ethylene terephthalate), Dr. Kevin McElea - University of Delaware, Newark, DE 19711

90. SAXS of fiber-filled polymer composites, Dr. R. Ullman - Ford Motor Company, Dearborn, MI 48121

91. SAXS studies on the deformation of segmented block polymers, Dr. Edwin L. Thomas - University of Massachusetts, Amherst, MA 01003

92. SAXS of controlled crystallized samples of linear polyethylene, Dr. L. Mandelkern - Florida State University, Tallahassee, FL 32306

93. Deformation studies of polyimide, Dr. T. P. Russell - IBM Research Laboratories, San Jose, CA 95193

94. Small-angle x-ray scattering studies of the morphology of plasticized P.V.C., Dr. H. R. Brown - Case Western Reserve University, Cleveland, OH 44106

95. Small-angle scattering from single phase diblock copolymers, Dr. F. S. Bates - Bell Laboratories, Murray Hill, NJ 07974

96. Effect of filler on molecular configuration in elastomers, Dr. C. M. Roland - Firestone Tire & Rubber Co., Akron, OH 44317

97. Kinetics, morphology, and mechanism of crystallization of poly(bistrifluoroethoxy phosphazene) in the region of T(1) transition, Dr. J. H. Magill - University of Pittsburgh, PA 15261

98. SAXS and SANS from carbon black filled polymers, Dr. Nigel Farrar - Raychem Corporation, Menlo Park, CA 94025

99. Small-angle x-ray scattering study of solution-crystallized polyethylene terephthalate, Dr. Leslie J. Fina - Case Western Reserve University, Cleveland, OH 44106

100. The effect of aging and thermal history on cluster formation in sulfonated polystyrene, Dr. Robert A. Weiss - University of Connecticut, Storrs, CT 06268

APPENDIX E

Publications and papers presented at scientific meetings by users and staff of the NCSASR.

LIST OF PUBLICATIONS AND PAPERS

R. K. Abele, G. W. Allin, W. T. Clay, C. E. Fowler, and M. K. Kopp, "Large-Area Proportional Counter Camera for the U. S. National Small-Angle Neutron Scattering Facility," IEE Transactions on Nuclear Science NS-28, 811 (1981).

W. W. Adams, T. E. Helminiak, A. Viswanathan, W. F. Hwang, and D. R. Wiff, "Molecular Composites: The Morphology of Rigid Rod/Random Coil Polymer Blends," p. 828 in Proceedings of the International Union of Pure and Applied Chemistry 28th Macromolecular Symposium, Amherst, MA, July 1982.

Hassan Bodaghi, "Spin-Drawn Interaction Effect on Fibrillation of Polypropylene," thesis, University of Tennessee, March 1982.

S. Babajko and J. M. Schultz, "Kinetics of Microstructure Rearrangement During Annealing of Cold-Drawn Isotactic Polypropylene," J. Polym. Sci. - Polym. Physics 20, 497-508 (1982).

F. S. Bates, C. V. Berney, R. E. Cohen, and G. D. Wignall, "Single-Chain Scattering in Heterogeneous Block Copolymers," Polymer (submitted).

F. S. Bates, R. E. Cohen, and C. V. Berney, "Small-Angle Neutron Scattering Determination of Macrolattice Structure in a Polystyrene-Polybutadiene Copolymer," Macromolecules 15, 589 (1982).

D. Bendedouch, S. H. Chen, W. C. Koehler, and J. S. Lin, "A Method for Determination of Inter-Particle Structure Factor of Macroions in Solution from Small-Angle Neutron and Light Scattering," J. Chem. Phys. 76, 10 (1982).

Dalila Bendedouch, Sow-Hsin Chen, W. C. Koehler, and J. S. Lin, "A Method for Determination of Intra- and Inter-Particle Structure Factors of Macroions in Solution from Small Angle Neutron Scattering," J. Chem. Phys. 76, 5022 (1982).

Dalila Bendedouch, Sow-Hsin Chen, and W. C. Koehler, "Structure of Ionic Micelles from Small Angle Neutron Scattering," J. Chem. Phys. (submitted 1982).

C. V. Berney, R. E. Cohen, and F. S. Bates, "Sphere Sizes in Diblock Copolymers: Discrepancy Between Electron Microscopy and Small-Angle Scattering Results," Polymer 23, 1222 (1982).

G. J. Bunick, E. C. Uberbacher, D. E. Olins, "Neutron Scattering and X-ray Diffraction of Nucleosomes and Nucleosome-HMG Complexes," The American Society of Cell Biology, Baltimore, MD, November 30 - December 4, 1982.

Bruce V. Ceres, "Electrical Breakdown in Polypropylenes," thesis, University of Delaware, August 1982.

H. R. Child and R. Triolo, "Small-Angle Neutron Scattering from Coal Extracts in Solution," American Physical Society Meeting, Dallas, TX, March 1982, [Bull. Am. Phys. Soc. 27, 292 (1982)].

H. R. Child, W. C. Koehler, J. S. Lin, L. Maddox, S. Spooner, V. Ramakrishnan, and G. D. Wignall, "The National Center for Small-Angle Scattering Research," Brookhaven Symposium in Biology No. 32, Upton, NY, May 31 - June 4, 1982.

D. K. Christen, W. C. Koehler, H. R. Kirchner, J. Narayan, S. T. Sekula, and Y. K. Chang, "Experimental Studies of Flux Line Lattice in Superconducting V_3Si," Symposium on Superconducting Materials, Materials Research Society, Boston, MA, November 1-4, 1982.

D. K. Christen, H. R. Kirchner, J. Narayan, B. C. Larson, S. T. Sekula, "Experimental Characterization of the Flux Line Lattice in Superconducting V_3Si," Conference on Applied Superconductivity, Knoxville, TN, November 30 - December 3, 1982.

S. Clough, D. Cortelek, T. Nagabhushanam, and J. Salamone, "Small Angle Neutron Scattering from an Ionomer," [Bull. Am. Phys. Soc. 27, 331 (1982)].

Buckley Crist and William Graessley, "SANS Studies of Model Crystalline Polymers," p. 656 in Proceedings of the International Union of Pure and Applied Chemistry 28th Macromolecular Symposium, Amherst, MA, July 1982.

B. Crist and W. W. Graessley, "SANS by Model Crystalline Polymers" [Bull. Am. Phys. Soc. 27, 330 (1982)].

J. Elad and J. M. Schultz, "Isothermal Crystallization of Oriented Nylon 6.6 Fibers" [Bull. Am. Phys. Soc. 27, 356 (1982)].

J. Elad and J. M. Schultz, "Microstructural Rearrangement During the Heat-Treatment of Drawn Nylon-6.6 Fibers," J. Polym. Sci. - Polym. Phys. Ed. (submitted 1982).

Joseph Elad, "Microstructural Development in Nylon-6.6 Fibers," master thesis, University of Delaware, June 1982.

J. E. Epperson, B. A. Loomis, and J. S. Lin, "Quantitative Comparison of the Void Distribution in a beta'-Phase Ni-Al-In Alloy Using X-Ray Small-Angle Scattering and Transmission Electron Microscopy," J. Nucl. Mater. 108-109, 476-484 (1982).

J. E. Epperson, B. A. Loomis, S. B. Gerber, G. H. Lander, J. S. Lin, R. W. Hendricks, and M. B. Lewis, "The Small-Angle X-Ray Scattering from Voids in Ion-Bombarded Nb," The AIME Meeting, Atlanta, GA, March 4-10, 1983

F. Fatemi, C. S. Paude, M. A. Imam, P. G. Moore, and H. R. Child, "Non-destructive Detection of a Pre-Omega Phase in Beta-III Ti by SANS," AIME Meeting, St. Louis, MO, October 14-20, 1982.

M. Fatemi, M. A. Imam, B. B. Rath, and H. R. Child, "Void Detection in Powder Consolidates and Superplastically Deformed Alloys by Long Wave-Length Neutrons," 111th AIME Annual Meeting, Dallas, TX, February 14-18, 1982.

R. L. Fellows and M. H. Lloyd, "The Use of Small Angle X-ray Scattering (SAXS) to Determine Particle Size: Application of Gel-Sphere Derived Reactor Fuel Preparation," The 84th Annual Meeting of the American Ceramic Society, Cincinnati, OH, May 1982.

R. L. Fellows and M. H. Lloyd, "The Use of Small Angle X-ray Scattering (SAXS) to Determine Particle Size: Application of Gel-Sphere Derived Reactor Fuel Preparation," J. Am. Ceramic Soc. 61, 383(1982).

R. L. Fellows and M. H. Lloyd, "The Determination of Crystallite Particle Sizes in Gel-sphere-Derived Reactor Fuel," 6th Actinide Separation Workshop, Augusta, GA, May 1982.

G. Hadziioannou, L. H. Wang, R. S. Stein, and R. S. Porter, "Small-Angle Neutron Scattering Studies on Amorphous Polystyrene Oriented by Solid State Coextrusion," Macromolecules 15, 880-882 (1982).

G. Hadziioannou, L.-H. Wang, R. S. Stein, and Roger S. Porter, "Neutron Scattering Studies of Polymer Deformation and Relaxation" [Bull. Am. Phys. Soc. 27, 331 (1982)].

H. G. Haubold and J. Lin, "Helium Bubbles in Nickel: A Small-Angle X-ray Scattering Study," Fifth International Conference on Plasma Surface Interactions in Controlled Fusion Devices, Gatlinburg, TN, May 1982.

H. G. Haubold and J. S. Lin, "He Bubbles in Ni: A Small-Angle X-ray Scattering Study," J. Nucl. Mater. (submitted).

H. Hayashi and P. Flory, "Configuration of the Polyisobutylene Chain in Bulk and in According to Elastic Neutron Scattering," Yamada Conference on Neutron Scattering of Condensed Matter, Hakone, Japan, September 1982.

R. W. Hendricks, S. Suehiro, and J. S. Lin, "Recent Progress in the Development of a Dynamic Device for the Study of the Plastic Deformation of Polymers," [Bull. Am. Phys. Soc. 27, 357 (1982)].

W. F. Hwang, C. L. Benner, and D. R. Wiff, and T. E. Helminiak, "Molecular Composites: Phase Relationships, Processing and Properties of Rod/Coil Polymer Blends," p. 827 in Proceedings of the International Union of Pure and Applied Chemistry 28th Macromolecular Symposium, Amherst, MA, July 1982.

W. F. Hwang, D. R. Wiff, C. L. Benner, and T. E. Helminiak, "Composites on A Molecular Level: Phase Relationships, Processing and Properties," Macromolecular Sci. Phys. (in press).

C. C. Koch, D. M. Kroeger, J. S. Lin, J. O. Scarbrough, W. L. Johnson, W. M. Keck and A. C. Anderson, "The Effect of Annealing on the Structure of an Amorphous $(Mo_{0.6}Ru_{0.4})_{82}B_{18}$ Alloy," Phys. Rev. B. (submitted).

W. C. Koehler, "The National Center for Small-Angle Scattering Research," American Physical Society, Phoenix, Arizona, March 16-20, 1981, [Bull. Am. Phys. Soc. 26, 400 (1982)] (invited paper).

W. C. Koehler, "Neutron Scattering Review - Magnetic Studies," Conference on the Neutron and Its Applications, Cambridge, England, September 13-17, 1982 (invited paper).

P. Krautwasser, "Study of Small-Angle X-ray Scattering from German Silicon Carbide Coatings," ORNL/GCR-82/4.

P. Krautwasser, G. M. Begun, and W. Kalf, "Characterization of SiC-Archive Batches A-834 through A-837 Included in Test HT-34," ORNL/GCR-82/8 and KFA-IRW/TN-23/82.

R. J. Lauf and P. Krautwasser, "Characterization of German Silicon Carbide Coatings," ORNL/GCR-81/13.

J. S. Lin, R. W. Hendricks, J. M. Shultz, and M. J. McCready, "Absolute Integrated SAXS Measurements During the Crystallization of Linear Polyethylene," J. Polymer Science 20, 1365 (1982).

J. S. Lin, W. C. Koehler, H. R. Child, G. D. Wignall, S. Spooner, and V. R. Ramakrishnan, "Research Facilities and Activities at the National Center for Small-Angle Scattering Research," The American Crystallographic Association Meeting, August 1982.

L. J. Magid, R. Triolo, J. S. Johnson, Jr., and W. C. Koehler, "Small-Angle Neutron Scattering Measurements on Micellar Solutions of Sodium Alkylbenzenesulfonates Having Branched Alkyl Groups," J. Phys. Chem. 86, 164 (1982).

J. G. Cabanas-Moreno, M. S. Yang, J. R. Weertman, M. Roth, Z. Y. Zhang, G. D. Wignall, and W. C. Koehler, "Studies of Grain Boundary Cavitation by Small-Angle Neutron Scattering," in Proc. ASTM Conf. on Quantitative Measurement of Fatigue Damage, (in press).

J. M. O'Reilly, D. M. Teegarden and G. D. Wignall, "Small-Angle Neutron Scattering (SANS) of Stereoregular Poly(methyl methacrylate) (PMMA)," American Chemical Society Northeast Regional Meeting, October 18-21, 1981, Rochester, New York [Bull. Am. Phys. Soc. 27, 330 (1982)].

James M. O'Reilly, "Molecular Structure and Dynamics of Stereoregular Poly(Methyl Methacrylate)," p. 527 in Proceedings of the International Union of Pure and Applied Chemistry 28th Macromolecular Symposium, Amherst, MA, July 1982.

R. A. Page, "Small Angle Neutron Scattering Measurements of Creep Damage in Structural Metals and Ceramics," The AIME Meeting, Atlanta, GA, March 4 - 10, 1983.

C. M. Roland, G.G.A. Bohm, and G. D. Wignall, "Shear Induced Coalescence of Domains in Heterogeneous Polymer Fluids," Polymer Preprints 23, 63 (1982).

Dale W. Schaefer, K. D. Keefer, and C. J. Brinker, "Characterization of Polymers and Gels by Intermediate-Angle X-ray Scattering," p. 490 in Proceedings of the International Union of Pure and Applied Chemistry 28th Macromolecular Symposium, Amherst, MA, July 1982.

R. S. Stein, G. Hadziioannou, and J. Gilmer, "Scattering Studies of Polymer Blends," [Bull. Am. Phys. Soc. 27, 331 (1982)].

R. S. Stein, "Recent Scattering Studies of Polymer Blends," p. 663 in the Proceedings of the International Union of Pure and Applied Chemistry 28th Macromolecular Symposium, Amherst, MA, July 1982 (invited paper).

S. Suehiro, R. W. Hendricks, and J. S. Lin, "Recent Progress in the Development of a Dynamic Device for the Study of the Plastic Deformation of Polymers," The American Physical Society, Dallas, TX, March 1982 [Bull Am. Phys. Soc. 27, 357 (1982)].

R. Triolo, L. J. Magid, J. S. Johnson, Jr., and H. R. Child, "Small-Angle Neutron Scattering from Aqueous Micellar Solutions of a Non-ionic Surfactant as a Function of Temperature," J. Phys. Chem. (submitted 1982).

E. C. Uberbacher, D. E. Olins, and G. J. Bunick, "Neutron Scattering Studies and Modeling of the HMG14 Core Nucleosome Complex," The American Crystallographic Association Meeting, San Diego, CA., August 1982.

E. C. Uberbacher, D. E. Olins, and G. J. Bunick, "Neutron Scattering Studies and Modeling of the HMG14 Core Nucleosome Complex," Brookhaven Symposium in Biology No. 32, Upton, NY, May 32 - June 4, 1982.

Edward C. Uberbacher, James K.W. Mardian, Randall M. Rossi, Donald E. Olins, and Gerard J. Bunick, "Neutron Scattering Studies annd Modeling of High Mobility Group 14 Core Nucleosome Complex," Proc. Natl. Acad. Sci. 79, 5258-5262 (1982).

J.W.C. Van Bogart, S. L. Cooper, and P. E. Gibson, "Small-Angle X-Ray Scattering Studies of Thermally-Induced Morphological Changes in Segmented Polyurethane Elastomers," [Bull. Am. Phys. Soc. 27, 168 (1982)].

Martin Paul Wai, "Small-Angle Scattering Studies of Isotactic and Atactic Polystyrene Blends," thesis, University of Massachusetts, December 1982.

J. R. Weertman, "Studies of Deformation Induced Grain Boundary Cavitation," The AIME Meeting, Atlanta, GA, March 4-10, 1983.

Paul A. Westbrook, "Morphological Studies of Polystyrene Crazes Using Small Angle X-ray Scattering," thesis, University of Tennessee, August 1982.

P. A. Westbrook, J. F. Fellers, R. W. Hendricks, and J. S. Lin, "Small-Angle X-ray Scattering Studies of Crazed Glassy Polymers," The American Physical Society, Dallas, TX, March 1982 [Bull. Am. Phys. Soc. 27, 197 (1982)].

D. R. Wiff, W.-F. Hwang, and W. W. Adams, "Small-Angle X-Ray Scattering Studies of A Rigid Rod/Flexible Coil Polymer Blend" [Bull. Am. Phys. Soc. 27, 297 (1982)].

G. D. Wignall, "Small-Angle Diffraction Studies of Synthetic Polymers at Oak Ridge," Pittsburgh Diffraction Conference, Cleveland, Ohio, November 4-6, 1981 (invited paper).

G. D. Wignall, H. R. Child, F. S. Bates, R. E. Cohen, C. V. Berney, and R. J. Samuels, "Structural Characterization of Phase Separated Polymer Blends by Small-Angle Neutron Scattering," p. 654 in Proceedings of the International Union of Pure and Applied Chemistry 28th Macromolecular Symposium, Amherst, MA, July 1982 (invited paper).

G. D. Wignall, "Small Angle Neutron Scattering from Synthetic Polymer at Oak Ridge," p. 24 in Proceedings of the International Union of Pure and Applied Chemistry 28th Macromolecular Symposium, Amherst, MA, July 1982.

G. D. Wignall, H. R. Child, F. S. Bates, R. E. Cohen, C. V. Berney, and R. J. Samuels, "Structural Characterization of Phase Separated Polymer Blends by Small-Angle Neutron Scattering," [Bull. Am. Phys. Soc. 27, 331 (1982)].

G. D. Wignall, H. R. Child, R. J. Samuels, "Structural Characterization of Semicrystalline Polymer Blends by Small-Angle Neutron Scattering," Polymer 23, 957 (1982).

G. D. Wignall, H. R. Child, W. C. Koehler, J. S. Lin, and R. L. Schmidt, "Small-Angle Scattering Studies of Pore Dimensions and Anisotropy in Shales," Geology (submitted).

M. H. Yoo, J. C. Ogle, J. H. Schneibel, and R. W. Swindeman, "Small Angle Neutron Scattering Study of Creep Deformation and Fracture of Type 304 Stainless Steel," Proceedings of the 6th International Conference on Strength of Metals and Alloys, Melbourne, Australia, August 16-20, 1982, Pergamon Press (in press).

M. H. Yoo, J. C. Ogle, I.-Wei Chen, and J. H. Schneibel, "Deformation-Induced Grain Boundary Cavitation - A Small-Angle Neutron Scattering Study," The AIME Meeting, Atlanta, GA, March 4-10, 1983.

P. Young, T. Kyu, S. Suehiro, J. S. Lin, and R. S. Stein, "Dynamic Small-Angle X-ray Scattering from Crystalline Polymers," J. Polymer Sci. - Polymer Phys. Ed. (submitted).

P. Young, T. Kyu, S. Suehiro, J. S. Lin, and R. S. Stein, "Dynamic Small-Angle X-ray Scattering from Crystalline Polymer," [Bull. Am. Phys. Soc. 27, 296 (1982)].

8.5 Oak Ridge Electron Linear Accelerator (ORELA)

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

Answer: The Oak Ridge Electron Linear Accelerator (ORELA) is a pulsed neutron time-of-flight spectrometry installation. It allows experimenters to obtain good results for a variety of types of measurements for neutron energies from 10^{-3} eV up to over 50 MeV. This facility provides the opportunity for a physicist to study in great detail the low spin states within a range of excitation energy equal to the neutron separation energy up to a few MeV above this point. Through this window one can observe in detail the characteristics of nuclear energy levels, their spacings, and their patterns of decay and thereby investigate reaction mechanisms and nuclear structure.

In recent years, new investigations have been directed to the optical model and collective excitation modes and to patterns of nuclear doorway states. The research questions asked change as advances are made with use of other probes and as theoretical ideas emerge.

This machine is an ideal tool for exploration of neutron capture cross sections to test the concepts of nucleosynthesis in stellar environments. While cross sections of about 150 nuclides have been measured throughout the important keV energy range, new subtle effects continue to make nuclear astrophysics a rich field.

Finally, this facility provides the most favorable applied science opportunities for studying with precision the cross sections of most importance in all aspects of nuclear technology. Most of the cross sections important for current applications have been measured to acceptable accuracy, but new applications for which only fragmentary information is available continue to arise. Moreover, for those nuclides of greatest practical importance, where one must know precise values of cross sections for optimal design and efficient operation of proposed facilities, a great deal of effort is yet required. The most successful new applied science is the use of high resolution gamma-ray spectrometry for the study of tertiary reactions of neutrons with energies above 10 MeV. Often, data of importance for the understanding of nuclear structure is gained through this applied work, as in the case of detailed low noise studies of the resonance structure in subthreshold fission.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

Answer: The important, unique features of the ORELA facility have been (1) high intensity, 10^{14} fast neutrons per second at the highest repetition rate, (2) highly flexible pulse repetition rate, (3) variable pulse width from 4 to 50 ns, (4) simultaneous use of up to 10 flight paths, (5) low counting background because of careful design and underground flight paths and stations, (6) narrow neutron energy resolution because of the combination of flight stations available and the detector and electronic equipment that permit their proper exploitation, (7) data acquisition and analysis computer systems that have functioned beautifully but are now obsolete and need to be replaced, and (8) an electrical grounding system developed at considerable effort that has controlled electrical interference problems which could render useless any detector producing low level signals.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

Answer: Neutron cross section experiments typically require from one week to several months of beam time. Productivity is enhanced by performing multiple experiments. This pattern places a premium on simple equipment that can operate reliably for long periods with daily surveillance and automatic recording.

The capabilities of the facility are not centered around a single spectrometer or a few spectrometer systems. Typical detection instruments are: (1) large gadolinium-loaded liquid scintillator for detection of neutron multiplicity following fission, (2) very large liquid scintillator for high efficiency neutron capture detection, (3) standardized capture cross section system using nonhydrogenous detectors with pulse height weighting and with an installed lithium glass neutron flux monitor (several similar facilities with slightly different capabilities have been used in recent years); (4) sample changers at both room temperature and liquid nitrogen temperature for transmission measurements, (5) lithium-drifted germanium detectors appropriately shielded against scattered neutrons for observations of reaction or capture gamma rays, (6) scattering chamber with multiple detectors for use in angular distribution measurements essential to the determination of spin and parity of resonances, (7) a variety of reliable flux monitors based on the boron, lithium, and hydrogen standard cross sections, (8) several carefully designed scintillator-based flux detectors appropriate for high resolution cross section measurements over a broad dynamic range, (9) fission ionization chambers containing a number of thin samples of each of several fissionable nuclides, (10) a variety of massive neutron collimators and associated beam handling equipment, (11) a variety of data analysis packages frequently used for derivation of fundamental parameters from the experimental data obtained.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer: The following are research highlights for the period FY 1981 to the present:

1. Measurement of the number of neutrons per (spontaneous) fission for ^{252}Cf to a well-justified 0.2% uncertainty.

2. Measurement of the energy dependence of the number of neutrons per fission from ^{239,241}Pu and ^{233,235}U over the region below 1 eV and the region from a few keV to a few MeV, all to a fraction of a percent uncertainty averaged over an application-dependent spectrum.

3. Transmission experiments using many samples of ^{238}U, exhaustive analyses, to define a precise representation of the cross section of this important isotope in the resonance region.

4. Measurement of subthreshold and threshold fission cross sections with high resolution for ^{232}Th, ^{238}U, ^{240}Pu, and ^{231}Pa. This has allowed examination of the detailed resonance structure as well as the shape and magnitude of the threshold.

5. Completion of studies of most stable fission product isotope capture cross sections to facilitate systematic study of fission product capture in fast reactors.

6. Fission cross section measurements of several highly radioactive higher actinide nuclides using a novel fission chamber design to suppress noise caused by alpha particles from natural decay. Previously unmeasurable resonance behavior was observed.

7. Demonstration of capability for total inelastic scattering measurements based on gamma-ray spectrometry, including definition of tertiary and higher order reaction products from the gamma-ray spectra.

8. Completion of a theoretical analysis leading to a consistent treatment of so-called statistical and systematic uncertainties in physical measurements based on a group theoretical treatment.

9. Successful application of pace-setting resonance analysis procedures to the analysis of ORELA-type data using techniques not previously applied based upon correct formulation of the resonance analysis and the so-called Bayesian approach.

10. Determination of the l-dependence of scattering from medium weight nuclides for various resonances, relative to calculations using a spherically symmetric optical model.

11. Measurements of total cross sections and the angular distribution of elastic neutron scattering for several nuclides of medium weight through the resonance region to determine spins and parities to elucidate doorway state patterns.

12. Measurement and analysis of the total cross sections of ^{86}Kr + n and ^{136}Xe + n and the interpretation of the delayed neutron spectra from ^{87}Br and ^{137}I to obtain beta-strength distributions.

13. Development of a more general nuclear reaction model in which spins are handled consistently even for multistep reactions involving both preequilibrium and equilibrium reactions. This model allows treatment in a logically consistent manner of the observed forward-biased angular distribution in preequilibrium reactions.

Expected output in the next 18 months includes (1) high resolution capture measurements on ^{238}U to allow identification of resonances seen in transmission up to the 10 keV level, (2) observation of precise ^{239}Pu fission cross sections to clarify discrepancies between experimental data and the data files used for practical applications, (3) completion of reaction gamma-ray observations on many nuclides up to 20 MeV neutron energy or above to determine inelastic scattering behavior and the presence of tertiary reactions to other than ground state, (4) observation of neutron emission spectra using a novel scintillation detector employing both time and pulse height observations to measure neutron angular and energy distributions, (5) completion of definitive sets of measurements of the nuclides in stainless steel and analysis of these data to provide realistic parameterization of these important cross sections. This includes the elimination of discrepancies in the previous analysis of the low-lying resonances in ^{56}Fe and zirconium that are important for neutron capture in these materials.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: Flight Path No. 3 was fitted with the standard equipment (collimators and beam stop) to permit its use for additional experiments.

The new Electron Beam Injector Laboratory, an addition to the second floor of the facility, is expected to be completed within the next fiscal year. The performance of ORELA has been found to be limited primarily by the performance of the injector, and adequate space for the assembly and test of injector components will then be available.

With the expected FY 1985 capital equipment funds, the ORELA Immediate Analysis Computer System is to be replaced. The existing computer is over 12 years old. Repairs are becoming difficult, and the computer is no longer sufficiently powerful to handle current demands.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer:

Oak Ridge Electron Linear Accelerator
(B/A in thousands of dollars)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operations					
Nuclear Sciences	$ 1,261	$ 1,443	$ 1,546	$ 1,600	$ 1,650
Research					
Nuclear Sciences	$ 947	$ 1,185	$ 1,363	$ 1,520	$ 1,765
Nuclear Physics	40	45	50	50	50
Magnetic Fusion Energy	0	31	36	40	43
Nuclear Energy	1,008	980	856	756	200
Equipment					
Nuclear Sciences	$ 153	$ 154	$ 154	$ 180	$ 500
Nuclear Energy	57	67	17	0	0
GPP					
Magnetic Fusion Energy	$ 0	$ 0	$ 340	$ 0	$ 0

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer: The Defense Nuclear Agency has been providing $30,000 per year for maintenance and upgrade of the Evaluated Nuclear Data File/Version B (ENDF/B) data files for which they have accepted responsibility.

8. For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.

Answer:

Oak Ridge Electron Linear Accelerator
(Staffing Levels in FTE's)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operations	12.2	13.2	14.7	14.7	12.2
Research	29.8	28.6	26.0	25.8	24.5

9. What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?

Answer: For the period FY 1981 - FY 1985, actual and estimated utilization of the Oak Ridge Electron Linear Accelerator facility is given in the following table:

ORELA Utilization

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Beam Hours for Research	4,770	3,610	3,110	4,300	4,700

We estimate full utilization to be 5,700 beam hours for research per year.

10. For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?

Answer: The number of experiments that have been run or are projected to be run in the period FY 1981 - FY 1985 is given below.

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Number of Experiments	23	25	24	27	19

Since a typical experiment is completed in less than a year's time, the number of experiments started and completed in each year is very nearly the same as shown in the table above.

11. What is this facility's user policy?

Answer: The Oak Ridge Electron Linear Accelerator (ORELA) is listed by the Laboratory as a "user facility" because it is available to users. However, the nature of research of ORELA, which normally involves a long time commitment for experiments and for analysis of detailed data, leads to the situation where essentially all users have collaborated with an ORNL researcher who is performing continuing work toward objectives similar to those of the outside user. For this reason, there is no committee of users that sets schedules or advises management on policy.

Potential users of ORELA are asked to discuss their interest with a staff member doing similar work. Usually, this contact is automatic and requests originate in this manner. If the Oak Ridge National Laboratory (ORNL) staff member is interested in the project, mutually convenient plans are set, consistent with other scheduling needs for the facility. In most cases, the outside user employs the equipment and the analysis programs normally used by his host, at least for the initial stages of data analysis.

Any request quite different from on-going work would come through ORELA management. We would accommodate the request if feasible. On a few occasions, we have suggested another facility which could perform the work more economically, e.g., experiments that require direct use of electron beams.

In at least one case, an outside group performed a series of experiments at ORELA with no local collaborator and only some interaction with ORELA management to facilitate the work of the group and to assure personnel safety.

12. For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?

Answer: The only reimbursable research that has taken place at the Oak Ridge Electron Linear Accelerator during this period has been done for the Defense Nuclear Agency.

Defense Nuclear Agency Reimbursables
(dollars in thousands)

FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
$ 28	$ 27	$ 37	$ 38	$ 32

13. What is the mechanism by which specific research proposals for experiments at the facility are considered?

Answer: If an Oak Ridge Electron Linear Accelerator (ORELA) staff member is interested in an experimental project and the sponsor concurs, an effort is made to schedule the experiment. All such proposals are studied by ORELA management prior to execution; the research programs are approved by management. In some cases, of course, the ideas for the research topics originate from management or from the Department of Energy.

In some cases, informal internal groups review the idea for a new type of experiment to weed out possible sources of difficulty. In a few cases, if the type of research proposed is somewhat different from traditional ORELA research, formal proposals are prepared and have been sent out for peer review.

In the case of work specifically designed to meet the needs of a particular nuclear technology, research goals are often defined by multilaboratory groups. In these cases, the needs-assessment groups usually do not comment on the techniques to be used for determining the values of needed cross sections.

14. How many research proposals have been submitted over the past five years, and how many of these have been approved?

Answer: Formal proposals for beam time at ORELA are not required from members of the ORELA staff. Outside users during the past five years have all worked in collaboration with ORELA staff and have not submitted proposals for beam time.

15. How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?

Answer: The following table shows the recorded number of university faculty and students that have used the facility.

Year	Number
1979	6
1980	4
1981	7
1982	5
1983	5

16. How many industrial researchers have utilized the facility over the past five years?

Answer: None.

17. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer: The table below shows the recorded numbers of non-U.S. researchers who have utilized the ORELA.

Year	Number
1979	7
1980	10
1981	7
1982	4
1983	9

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: None.

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: Generic development possibilities at ORELA include reliability improvement, power increases, shortening of the electron pulses at maximum beam power, narrowing ultimate resolution by flight path lengthening or target thinning, beam geometry improvement, major detector additions, updated data acquisition and analysis equipment. Current plans in these areas are listed below.

Accelerator reliability improvement:

The Electron Beam Injector Laboratory, a second floor addition, is presently funded at $0.34M as a FY 1983 ORNL General Plant Project. It is expected to be completed by late FY 1985. That area will be used for electron gun protection and improved test devices that should allow us to improve electron gun reliability and projected performance in later years.

Power Increases:

An investigation has been underway to see how the klystrons used at ORELA could be upgraded to have the higher efficiency characteristics of more modern klystrons. Through a partial redesign it should be possible to obtain higher power output with less input power and correspondingly lower maintenance of the "modulators" used to drive the klystrons.

Shortening electron beam pulses at maximum beam power:

This is accomplished by increasing peak electron current. The "klystron prebuncher apparatus" installed four years ago has not improved injector performance as anticipated. It is being removed to allow analysis of the performance data obtained using it, the accuracy of the theoretical calculations originally used in its design, and its potential for modification to achieve the high-intensity short pulses originally sought.

Beam geometry improvement:

The sample changer apparatus on the prime 200 m flight path is being altered to allow the sample to be placed at 80 m. This will enhance counting rates and permit better monitoring of the beam intensity in transmission experiments.

20. Please provide a copy of the facility's latest annual report.

Answer: The ORELA does not produce an annual report; however, almost all the research performed is covered in the Annual Report of Engineering Physics and Mathematics Division (ORNL-6030), published in March 1984 and a copy of the pertinent section is attached.

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ENGINEERING PHYSICS DIVISION PROGRESS REPORT PERIOD ENDING DECEMBER 31, 1983

F. C. Maienschein, Director

Date Published - March 1984

Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831
operated by
Union Carbide Corporation
for the
Department of Energy

1.0. INTRODUCTION

A decade ago the research performed at the Oak Ridge Electron Linear Accelerator (ORELA) was split about evenly between the ORNL Physics Division and the Engineering Physics Division, the former group emphasizing studies of nuclear structure and neutron reaction mechanisms and the latter devoting more effort toward obtaining precise values of the cross sections needed for the nuclear energy programs. Over the years the emphasis has shifted toward the practical needs. In the fall of 1982, over one-half of the ORELA research being reported through the Physics Division was transferred to our division. The shifted research includes capture cross-section measurements motivated by astrophysical interests; measurements of neutron capture by fission products needed for fast reactor design; detailed high-resolution studies of resonance structure crucial to the determination of level densities and spacing distributions; fission cross sections of heavy alpha-active actinides; and total cross sections over a very broad incident-neutron energy range and for a number of elemental and isotopic samples to study variations in neutron strength versus energy, atomic mass, and angular momentum. Much of this work has included efforts of many visiting scientists from universities and national laboratories in the U.S. and in foreign countries.

Many aspects of the transferred research bear on the development of files of evaluated nuclear data for applied needs and so fit neatly into the established patterns of the division. Other aspects, however, will require a broadening of our scope to include research designed primarily to enhance understanding of physics.

Considerable leadership effort continues within our nuclear data groups to establish useful and correct techniques for codification of the variance-covariance matrix of experimental as well as "evaluated" results. ORELA experiments typically involve thousands or tens of thousands of data points, so correct representation of the covariances among the data elements is challenging. In several cases, we have now achieved adequate success. As publication of experimental results is accompanied by rational and complete expressions of experimental uncertainties, correct combination of experimental results from various sources to obtain evaluated data files will have a more solid (scientific) basis. Indeed, we have now reached the point in neutron cross-section research where only well conceived, executed, and documented experimental results are justifiable for public support. A careful report of uncertainties and correlations is required.

There has nearly always been a free international sharing of experimental neutron cross-section results. In addition, international collaboration on particular experimental research efforts frequently occurs. Such international cooperation has not been widespread in the generation and use of evaluated cross-section data files. However, the Nuclear Energy Agency Nuclear Data Committee, an international group, set a new pattern last year by appointing select committees to collaborate in depth toward resolving two important areas of discrepancy: (a) parameters of the 1.15-keV resonance in the ($n+{}^{56}$Fe) cross section and (b) the overall resonance parameterization of the ($n+{}^{238}$U) reaction above 1 keV. Members of our division are taking active leading roles on these committees, and the efforts are expected to be largely successful. This international effort originated in the recognition that, despite the great world knowledge of neutron nuclear data, some of the most important problems have not been resolved.

During recent years about one-third of our nuclear data research has been supported by the DOE fast reactor program. (One-fifth of accelerator costs are included.) With the cancellation of the Clinch River Breeder Reactor and the subsequent continuing program re-evaluations, it is uncertain how much emphasis in that program will be placed on technology improvements that have a several year time scale, such as the effort to establish a fully satisfactory fast reactor data base in the next (sixth) version of the ENDF/B nuclear data file. Much of the fast reactor nuclear data work across the country might be transferred to the DOE Office of Energy Research, which already supports most of the ORNL effort through its Basic Energy Sciences program. In the face of these uncertainties, we have cooperated at length during the past year in a multilaboratory effort to solidify and make more efficient the cross-section evaluation work (data combination and codification) that has been supported by the fast reactor program. A written plan has been developed to focus effort on the most important cross sections, taking into account planned new measurements and the evaluation work and review effort thought to be needed to provide fast reactor engineers with a cross-section data base adequate for the precise design of and eventual use of efficient fast reactors of any of the wide variety of types now being considered. The plan assumes a constant level of effort for a few years. Long-term efforts of the type discussed here are not carried out efficiently with irregular funding, so there is an urgency to avoid hasty budgetary changes that could destroy the effectiveness of the present program.

As was indicated in an earlier progress report, we performed some accelerator facility studies to determine whether accelerator design options now exist that would allow relatively economical replacement of ORELA with a 200- to 300-MeV proton accelerator. Members of the Accelerator Technology Division of Los Alamos National Laboratory helped our staff to perform these studies of linear accelerators. As expected, the results indicated that a proton accelerator could give significantly improved intensity for most of the experiments performed at ORELA, especially for those at neutron energies above several MeV. However, such an accelerator facility would require an investment of about $40M (1986 dollars). We concluded that an economical linac-based proton accelerator would not be an improvement over ORELA in its range of strong performance. No further work in this area is presently planned after the documentation of what has already been completed.

In the areas of ORELA operation and development, we have tried very hard to realize the long-established goal of bringing into routine use the "prebuncher" that was constructed to compress the ORELA charge pulse and thereby increase the intensity available for short-pulse experiments. Monitoring of the beam has been greatly improved and some definite obstacles have been identified and overcome; however, additional problems have recently been recognized and the goal to gain performance through routine prebuncher use has not been reached even though the apparatus has been operated without difficulty for periods longer than a day. The best results so far obtained with the prebuncher are not superior to the best ones logged in prior years before the prebuncher was installed. Goals for the near future are to determine whether the difficulties are fundamental and, if not, to discover how the design needs to be modified. Then the prebuncher will be removed and the identified improvements installed if such action seems warranted.

The abstracts reproduced in this first section, representing papers and reports published or accepted for publication since our last progress report and before January 1, 1984, reveal the diversity of our staff and missions. The first subsection includes abstracts of papers containing new experimental results — mostly from research performed at ORELA. The second subsection includes abstracts covering analyses of other experimental results, theoretical calculations, and various reviews of topics in our areas of expertise. The last subsection includes abstracts of papers dealing with techniques of measurement and analysis and with research facilities.

Measurements

1.1

NEUTRON CAPTURE IN THE 1.15-keV RESONANCE OF IRON[*]

R. L. Macklin

[Abstract of *Nucl. Sci. Eng.* 83, 309 (1983)]

A direct measurement of the capture area in the 1.1515 ± 0.0007 keV (^{56}Fe + n) resonance leads to $g\Gamma_n\Gamma_\gamma/\Gamma = 68.7 \pm 1.5$ MeV, $\sigma_0\Gamma_\gamma = 161 \pm 4$b-eV.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

1.2

NEUTRON CAPTURE IN s-WAVE RESONANCES OF ^{64}Ni[*]

K. Wisshak[†] F. Käppeler[†]
R. L. Macklin G. Reffo[‡]
F. Fabbri[‡]

(Abstract of KfK-3582, September 1983)

The neutron capture widths of the s-wave resonances at 13.9 and 33.8 keV in ^{64}Ni have been determined using a setup with extremely low neutron sensitivity completely different from all previous experiments on this isotope. This feature is important because these resonances exhibit a very large scattering to capture ratio. A pulsed 3-MV Van de Graaff accelerator and a kinematically collimated neutron beam, produced via the ^{7}Li(p,n) reaction, was used in the experiments. Capture gamma rays were observed by three Moxon-Rae detectors with graphite, bismuth-graphite, and bismuth converters, respectively. The samples were positioned at a neutron flight path of only 6-8 cm. Thus events due to capture of resonance scattered neutrons in the detectors or in surrounding materials are completely discriminated by their additional time of flight. The short flight path and the high neutron flux at the sample position allowed for a signal-to-background ratio of ~1 even for the broad resonance at 33.8 keV. The data obtained with the individual detectors were corrected for the efficiency of the different converter materials. For that purpose, detailed theoretical calculations of the capture gamma-ray spectra of the measured isotope and of gold, which was used as a standard, were performed. The final radiative widths are Γ_γ (13.9 keV) = 1.01 ± 0.07 eV and Γ_γ (33.8 keV) = 1.16 ± 0.08 eV, considerably smaller than the rough estimates obtained in previous work.

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[*] Research sponsored by Kernforschungszentrum Karlsruhe GmbH, Karlsruhe.

[†] Institut für Kernphysik, Karlsruhe.

[‡] Dell'Energia Nucleare e Delle Energie Alternative, Bologna, Italy.

1.3

RESONANCE NEUTRON CAPTURE IN ^{86,87}Sr[*]

G. C. Hicks[†] B. J. Allen[‡]
A. R. de L. Musgrove[†] R. L. Macklin

[Abstract of *Aust. J. Phys.* 35, 267 (1982)]

The neutron capture cross sections of ^{86,87}Sr have been measured with high energy resolution from 3 to 200 keV at the 40 m station of the Oak Ridge Electron Linear Accelerator. Individual resonances were analyzed to 37 keV for ^{86}Sr and to 14 keV for ^{86}Sr, and average resonance parameters were deduced on the basis of assumed divisions between s- and p-wave resonances. The average radiative widths obtained on this basis are consistent with a capture mechanism which is predominantly statistical.

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[*] Research sponsored by U.S. DOE Division of Physics.

[†] James Cook University of North Queensland, Townsville, Queensland, Australia.

[‡] Lucas Heights Research Laboratories, Sutherland, New South Wales.

1.4

TECHNETIUM-99 NEUTRON CAPTURE CROSS SECTION*

R. L. Macklin

[Abstract of *Nucl. Sci. Eng.* 81, 520 (1982)]

The ^{99}Tc(n,γ) average cross section was measured at the Oak Ridge Electron Linear Accelerator from 2.65 to 2000 keV with an estimated uncertainty ranging from 4.0 to 4.9%. Individual resonance parameters were fitted by least-squares adjustment to the capture yield data from 2.65 to 5.08 keV. The average cross-section data agree with the ENDF/B-V (Mod 1) evaluation above 900 keV and lie within ±15% of the JENDL-1 evaluation below 700 keV.

*Research sponsored by U.S. DOE Division of Nuclear Sciences.

1.5

NEUTRON CAPTURE CROSS SECTIONS OF THE SILVER ISOTOPES ^{107}Ag AND ^{109}Ag FROM 2.6 TO 2000 keV*

R. L. Macklin

[Abstract of *Nucl. Sci. Eng.* 82, 400 (1982)]

Prompt neutron capture from highly enriched samples of the stable silver isotopes was measured at the Oak Ridge Electron Linear Accelerator neutron time-of-flight facility. Resonance peaks were parameterized from 2.65 to 7 keV, and average capture cross sections were derived as a function of energy up to 2000 keV. The average values for the ^{109}Ag(n,γ) cross section are a few percent smaller than for ^{107}Ag up to 700 keV, above which energy they drop more rapidly, falling to ~60% of the ^{107}Ag(n,γ) cross section at 2000 keV. Average radiation widths found for spin 1 resonances were 152 ± 7 meV for ^{107}Ag and 146 ± 6 meV for ^{109}Ag. Maxwellian average cross sections for kT = 30 keV are 801 mb for ^{107}Ag and 778 mb for ^{109}Ag with estimated uncertainties of 3%.

*Research sponsored by U.S. DOE Division of Nuclear Sciences.

1.6

NEUTRON CAPTURE CROSS SECTIONS AND RESONANCES OF ^{127}I AND ^{129}I*

R. L. Macklin

[Abstract of *Nucl. Sci. Eng.* 85(4), 350 (1983)]

Neutron capture by ^{127,129}I has been measured using the Oak Ridge Electron Linear Accelerator (ORELA) as a pulsed neutron source. Neutron energies were determined by time-of-flight. Resonance peaks were parametrized for radioactive ^{129}I up to 3400 eV, and for stable ^{127}I from 2660 eV to 4260 eV. Average capture cross sections were derived for ^{129}I from 3 keV to 500 keV and for ^{129}I from 3 keV to 2200 keV. Over the 3 keV to 100 keV range, the ^{129}I cross sections average about 70% of the corresponding ^{127}I cross sections but show much more fluctuation as a function of energy. The greater fluctuation is attributed to the approximately three times wider level spacing.

*Research sponsored by U.S. DOE Division of Nuclear Sciences.

1.7

CESIUM-133 NEUTRON CAPTURE CROSS SECTION*

R. L. Macklin

[Abstract of *Nucl. Sci. Eng.* 81, 418 (1982)]

The ^{133}Cs(n,γ) cross section was measured at the Oak Ridge Electron Linear Accelerator from 2.66 to 600 keV with 3 to 4% uncertainty. Individual resonance parameters were determined by least-squares adjustment to fit the yield data below 6 keV and the average cross section was derived up to 600 keV.

*Research sponsored by U.S. DOE Division of Nuclear Sciences.

1.8

CROSS SECTIONS OF THE ^{169}Tm (n,γ) REACTION FROM 2.6 keV TO 2 MeV[*]

R. L. Macklin D. M. Drake[†]
J. J. Malanify[†] E. D. Arthur[†]
P. G. Young[†]

[Abstract of *Nucl. Sci. Eng.* 82, 143 (1982)]

Neutron capture cross sections have been measured for ^{169}Tm from 3 to 2000 keV at the Oak Ridge Electron Linear Accelerator 40-m station. The data were analyzed for individual resonance parameters up to 4.2 keV. Average strength functions have been deduced. Compound nucleus calculations, made with deformed optical model parameters, agree with experimental cross sections. Our cross sections for lower neutron energies tend to be somewhat less than those from earlier measurements.

[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

[†] Los Alamos National Laboratory, Los Alamos, NM.

1.9

^{178,179,180}Hf AND ^{180}Ta(n,γ) CROSS SECTIONS AND THEIR CONTRIBUTION TO STELLAR NUCLEOSYNTHESIS[*]

H. Beer[†] R. L. Macklin

[Abstract of *Phys. Rev. C* 26(4), 1404 (1982); paper presented at the International Conference on Nuclear Data for Science and Technology, Antwerp, Belgium, September 6 10, 1982; Proc. p. 945, K. H. Bockoff, Ed. (1983)]

The neutron capture cross sections of ^{178,179,180}Hf were measured in the energy range 2.6 keV to 2 MeV. The average capture cross sections were calculated and fitted in terms of strength functions. Resonance parameters for the observed resonances below 10 keV were determined by a shape analysis. Maxwellian averaged capture cross sections were computed for thermal energies kT between 5 and 100 keV. The cross sections for $kT = 30$ keV were used to determine the population probability of the 8^- isomeric level in ^{180}Hf by neutron capture as $(1.24 \pm 0.06)\%$ and the *r*-process abundance of ^{180}Hf as 0.0290 $(\mathrm{Si} = 10^6)$. These quantities served to analyze *s*- and *r*-process nucleosynthesis of ^{180}Ta.

[*] Research sponsored by U.S. DOE Division of Nuclear Sciences.

[†] Kernforschungszentrum Karlsruhe GmbH, Germany.

1.10

NEUTRON CAPTURE CROSS SECTIONS OF TANTALUM FROM 2.6 TO 1900 keV[*]

R. L. Macklin

(Abstract of *Nucl. Sci. Eng.*, in press)

Neutron capture by a tantalum sample was measured at the Oak Ridge Electron Linear Accelerator (ORELA) pulsed neutron time-of-flight facility on a 40 m flight path. Average cross sections for ^{181}Ta(n,λ) in the energy range from 2.6 to 1900 keV were derived. The partially resolved region from 2620 to 4000 eV was fitted in terms of resonance parameters by least squares adjustment.

[*] Research sponsored by U.S. DOE Division of Basic Energy Sciences.

1.11

NEUTRON CAPTURE CROSS SECTIONS OF ^{182}W, ^{183}W, ^{184}W, AND ^{186}W FROM 2.6 TO 2000 keV[*]

R. L. Macklin D. M. Drake[†]
E. D. Arthur[†]

[Abstract of *Nucl. Sci. Eng.* 84, 98 (1983)]

Neutron capture cross sections of four stable tungsten isotopes were measured as a function of energy by time of flight at the Oak Ridge Electron Linear Accelerator. The resolution achieved, $\Delta E/E$ of $\sim 1/750$ at full-width at half-maximum, has allowed the analysis of several hundred resonance peaks at energies a few kiloelectron volts above the neutron binding energy. Strength functions were fitted to the average cross sections up to ~ 100 keV, and average cross sections were extended with less precision from 100 to 2000 keV. The capture cross section of natural tungsten was calculated from measurements for individual isotopes. Compound nucleus calculations have been made with deformed optical model parameters for comparison with experimental cross sections.

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*Research sponsored by U.S. DOE Division of Nuclear Sciences.

[†] Los Alamos National Laboratory, Physics Division, Los Alamos, NM.

[‡] Los Alamos National Laboratory, Theoretical Division, Los Alamos, NM.

1.12

COMPARISON OF MEASURED AND CALCULATED ^{238}U CAPTURE SELF-INDICATION RATIOS FROM 4 TO 10 keV*

R. B. Perez G. de Saussure
J. T. Yang[†] J. L. Munoz-Cobos[‡]
J. H. Todd[§]

[Abstract of *Trans. Am. Nucl. Soc.* 44, 537 (1983); also paper presented at the Second Jackson Hole Colloquium on Fast Reactor Physics: The Doppler Effect in LMFBRs, Teton Village, Wyoming, June 27-29, 1983; Proc. Session III, No. 4 (1983)]

From 4 to 149 keV, the ^{238}U cross sections are represented in ENDF/B-V by unresolved-resonance parameters (URPs). The purpose of this representation is to enable the calculation of resonance self-protection as a function of temperature and dilution. Since the URPs are not defined unambiguously by the cross-section data, it is important that the unresolved representation be tested with appropriate experiments, such as capture self-indication ratio (SIR) measurements. In this paper, we compare ^{238}U capture SIR measurements in the 4- to 10-keV energy range with calculations done with ENDF/B-V and with recently published resolved-resonance parameters.

The above comparisons suggest that:

1. The measured ^{238}U capture SIR has a considerable amount of structure as a function of energy.
2. The ENDF/B-V unresolved-resonance representation fails to reproduce this structure.
3. Calculations done with available resolved-resonance parameters in the 4- to 6-keV interval reproduce the structure fairly well.
4. From 6.5 to 10 keV, ENDF/B-V underestimates resonance self-protection for the thicker samples.
5. Below 5.5 keV, ENDF/B-V overestimates resonance self-protection for the thin samples but is in agreement with the measurements for the thick samples.
6. Calculations based on resolved parameters agree significantly better with the measurements than those based on ENDF/B-V.

These considerations underscore the need to extend the ^{238}U resolved-resonance representation of ENDF/B to higher energies if the 1% accuracies in computed ^{238}U self-shielding factors requested by reactor designers is to be achieved.

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*Research sponsored by U.S. DOE Office of Reactor Research and Technology.

[†] Institute of Nuclear Research, Taiwan, Republic of China.

[‡] Universidad Politecnica de Valencia-Spain.

[§] Instrumentations and Controls Division.

1.13

OVERLAPPING β DECAY AND RESONANCE NEUTRON SPECTROSCOPY OF LEVELS IN ^{87}Kr*

S. Raman[†] B. Fogelberg[‡]
J. A. Harvey R. L. Macklin
P. H. Stelson[†] A. Schröder[§]
K. L. Kratz[§]

[Abstract of *Phys. Rev. C* 28(2), 602 (1983); also *Bull. Am. Phys. Soc.* 27(7), 727 (1982)]

Energy levels in ^{87}Kr have been studied, with special emphasis on the unbound region, using two different methods. The first method comprises neutron capture and transmission measurements on an enriched gas target of ^{87}Kr using neutron time-of-flight techniques. In this way, neutron widths were determined for 39 resonances below 400 keV and capture areas for 14 resonances below 90 keV. The second method is a decay study of 56-s ^{87}Br in which a level scheme for ^{87}Kr has been established that shows 126 levels in the bound and 12 levels in the unbound region. A detailed comparison amongst the neutron resonance, the γ-ray decay, and available delayed neutron results has been made.

Almost a one-to-one correspondence exists between the currently observed p-wave resonances below 250 keV and levels in ^{87}Kr studied through delayed neutron emission. The overall β-strength distribution derived from the present data shows broad resonance-like structures. However, no marked selectivity is observed in the β decay to individual levels in the unbound region of ^{87}Kr. The neutron capture cross section of ^{87}Kr is found to be about 5 mb for 30-keV neutrons with a Maxwellian energy distribution. The future of delayed neutron spectroscopy as a new tool for obtaining level-density information is discussed.

[*] Research sponsored by U.S. DOE Division of Nuclear Sciences.

[†] Physics Division.

[‡] Studsvik Science Research and Laboratory, Facks-611 01, Nykoping, Sweden.

[§] Institut für Kernchemie, Universität Mainz, D-65 Mainz, Federal Republic of Germany.

1.14

NEUTRON SPECTROSCOPY AS A HIGH-RESOLUTION PROBE: IDENTIFICATION OF THE MISSING $1/2^+$ STATES IN ^{31}SI*

J. A. Harvey W. M. Good[†]
R. F. Carlton[‡] B. Castel[§]
J. B. McGrory[†] S. F. Mughabghab[¶]

[Abstract of *Phys. Rev. C* 28(1), 24 (1983)]

The neutron total cross section of ^{30}Si$+n$ was measured from 0.2 to 1400 keV and the data were analyzed to obtain resonance parameters. Two s-wave resonances corresponding to $1/2^+$ states in ^{31}Si predicted from shell model calculations were found. Contrary to earlier (d,p) measurements, the present measurement indicates a fairly uniform fragmentation of p-wave strength, in agreement with earlier weak coupling shell model calculations of negative parity states for ^{29}Si and ^{33}S.

[*] Research sponsored by U.S. DOE Division of Nuclear Sciences.

[†] Physics Division.

[‡] Middle Tennessee State University, Murfreesboro, TN.

[§] Queen's University, Kingston, Ontario, Canada.

[¶] Brookhaven National Laboratory, Upton, NY.

1.15

SOLID STATE EFFECTS ON THERMAL NEUTRON CROSS SECTIONS AND ON LOW ENERGY RESONANCES*

J. A. Harvey H. A. Mook[†]
N. W. Hill[‡] O. Shahal[§]

[Abstract of paper presented at the International Conference on Nuclear Data for Science and Technology, Antwerp, Belgium, September 6-10, 1982; Proc. p. 961, K. H. Bockoff, Ed. (1983)]

The neutron total cross sections of several single crystals (Si, Cu, sapphire), several polycrystalline samples (Cu, Fe, Be, C, Bi, Ta), and a fine powder copper sample have been measured from 0.002 to 5 eV. The Cu powder and polycrystalline Fe, Be, and C data exhibit the expected abrupt changes in cross section. The cross section of the single crystal of Si is smooth with only small broad fluctuations. The data on two "single" Cu crystals, the sapphire crystal, cast Bi, and rolled samples of Ta and Cu have many narrow peaks $\sim 10^{-3}$ eV wide. High resolution (0.3%) transmission measurements were made on the 1.057-eV resonance in ^{240}Pu and the 0.433-eV resonance in ^{180}Ta, both at room and low temperatures to study the effects of crystal binding. Although the changes in Doppler broadening with temperature were apparent, no asymmetries due to a recoilless contribution were observed.

[*] Research sponsored by U.S. DOE Division of Nuclear Sciences.

[†] Solid State Division.

[‡] Instrumentation and Controls Division.

[§] Nuclear Research Centre-Negev, Beer-Sheva, Israel.

1.16

UNBOUND STATES OF ^{35}S AND DOORWAY STATE CALCULATIONS*

R. F. Carlton[†] J. A. Harvey
W. M. Good[‡] B. Castel[§]

[Abstract of *Bull. Am. Phys. Soc.* 27(7), 712 (1982)]

Total cross section measurements have been made on an enriched ^{34}S (90.0%) sample ($1/N_t = 10.79$) from 20 eV to 1.45 MeV using the 80-m flight path at ORELA. The measurements were made using a ^{6}Li glass scintillator up to ~50 keV and using a NE-110 scintillation detector above ~50 keV with an energy resolution of 0.1% below 250 keV and $0.2\%\sqrt{E(in\ MeV)}$ above 250 keV. The data were analyzed with the R-matrix multilevel code SAMMY to obtain resonance parameters for s-, p-, and d-wave neutrons. The s- and p-wave neutron widths were compared with a doorway state calculation using shell model parameters determined by a ^{35}Cl-^{35}S bound state calculation. Agreement with data is satisfactory enough to assign theoretical doorway state configurations to specific groups of resonances.

[*] Research sponsored by U.S. DOE Division of Nuclear Sciences.

[†] Middle Tennessee State University, Murfreesboro, TN.

[‡] Physics Division; Presently 113 Taylor Rd., Oak Ridge, TN.

[§] Queen's University, Kingston, Ontario, Canada.

1.17

APPLICATION OF NEW TECHNIQUES TO ORELA NEUTRON TRANSMISSION MEASUREMENTS AND THEIR UNCERTAINTY ANALYSIS: THE CASE OF NATURAL NICKEL FROM 2 keV TO 20 MeV*

D. C. Larson N. M. Larson[†]
J. A. Harvey N. W. Hill[‡]
C. H. Johnson[§]

(Abstract of ORNL/TM-8203, October 1983)

The neutron transmission through a 2.54-cm sample of natural nickel has been measured for neutron energies between 2 keV and 20 MeV. The Oak Ridge Electron Linear Accelerator (ORELA) was used to provide the neutrons which were detected at the 200-m flight path by a NE110 proton recoil detector. A selective rating system was utilized to minimize background effects due to large light-level events which produce phototube afterpulsing and long decay-constant light emission in the detector. A detailed discussion of the development of this system is given.

Known background sources are described, and the methods used to correct for these backgrounds are presented. An in-depth uncertainty analysis is given for this measurement, with explicit formulas derived for each effect contributing to the cross-section uncertainty. Parameter uncertainties and correlations among the parameters describing the backgrounds, deadtime, and other sources of uncertainty are given. To obtain a covariance matrix for this measurement, the final cross-section results are binned into 15 energy groups, and a covariance matrix is provided for this 15-group set. We find that the largest contributions to the cross-section uncertainty are due to sample properties, beam monitors (used to normalize sample-in and sample-out counts), and ORELA power variations during the run which affect the deadtime correction. Overall uncertainties in the cross section for this measurement are on the order of 2%. The resulting cross sections are compared with the ENDF/B-V file for nickel; any resonances not presently in the file are observed, and energy-scale differences are noted.

[*] Research sponsored by U.S. DOE Division of Basic Energy Sciences and Division of Reactor Research and Technology.

[†] UCC-ND Computer Sciences Division.

[‡] Instrumentation and Controls Division.

[§] Physics Division.

1.18

HIGH RESOLUTION NEUTRON TOTAL CROSS SECTION IN THE SEPARATED ISOTOPES OF ^{52}Cr AND ^{54}Cr*

H. M. Agarwal[†] J. B. Garg[†]
J. A. Harvey

[Abstract of *Bull. Am. Phys. Soc.* 27(7), 716 (1982)]

High resolution neutron total cross sections in the energy interval of 10-900 keV have been performed in the enriched isotopes of chromium with masses 52 and 54. These measurements were made with the ORELA facility using time-of-flight techniques. From these data, parameters (E, Γ_n, J^{π}) of s and p-wave resonances were obtained using an R-matrix multilevel analysis. Moreover we have investigated the statistical properties of level parameters such as neutron reduced width distribution, short and long range spacing distributions and neutron strength functions. A detailed discussion of these results is presented.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

[†] State University of New York-Albany.

1.19

HIGH RESOLUTION NEUTRON RESONANCE SPECTROSCOPY IN ^{89}Y[*]

H. M. Agarwal[†] J. B. Garg[†]
J. A. Harvey

[Abstract of *Bull. Am. Phys. Soc.* 28(4), 736 (1983)]

The neutron total cross section in ^{89}Y in the energy range of 10 keV to 800 keV has been measured using ORELA facility. R-matrix analysis of this high resolution data has provided values of E_o, Γ_n, J^π for s- and p-wave resonances. From these results the values of average resonance parameters such as level spacing and strength functions for s- and p-wave neutron interactions have been obtained. The s- and p-wave neutron reduced width distributions have also been studied. Moreover we have investigated $S_o(J^\pi = 0^-)$, $S_o(J^\pi = 1^-)$, $S_1(J^\pi = 0^+)$, $S_1(J^\pi = 1^+)$, $S_1(J^\pi = 2^+)$ vs. energy, respectively, in search of intermediate structures which were theoretically predicted by Ramavataram *et al.* A detailed discussion of these findings is presented.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

[†] State University of New York-Albany.

1.20

^{187}Os + *n* RESONANCE PARAMETERS IN THE INTERVAL 27-500 eV NEUTRON ENERGIES[*]

R. R. Winters[†] R. F. Carlton[‡]
J. A. Harvey N. W. Hill[§]

[Abstract of paper presented at the International Conference on Nuclear Data for Science and Technology, Antwerp, Belgium, September 6-10, 1982; Proc. p. 943, K. H. Bockoff, Ed. (1983)]

The neutron total cross section for ^{187}Os in the energy range 27 eV to 500 eV has been measured at the ORELA facility by the neutron time-of-flight technique, utilizing a 2.0 g osmium sample ($n = 0.008401$ Os-nuclei/barn) enriched to 70.38% ^{187}Os. Measurements were performed at a 80 m flight station with an energy resolution, $\Delta E/E$, of 0.1% using a ^{6}Li glass scintillator. Resolved resonances have been analyzed by a Reich-Moore multilevel code (SAMMY) to obtain parameters for 85 resonances up to 500 eV. Preliminary determinations of the level spacing (5 eV) and s-wave strength function (3.9×10^{-4}) for ^{187}Os are in agreement with recent analyses of the osmium isotopes, made in connection with the use of the Re/Os chronometer for estimating the duration of stellar nucleosynthesis.

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[*] Research sponsored by U.S. DOE Division of Nuclear Sciences.

[†] Denison University, Granville, OH.

[‡] Middle Tennessee State University, Murfreesboro, TN.

[§] Instrumentation and Controls Division.

1.21

THE TOTAL NEUTRON CROSS SECTIONS OF ^{249}Bk AND ^{249}Cf BELOW 100 eV[*]

R. W. Benjamin[†] J. A. Harvey
N. W. Hill[‡] M. S. Pandey[‡]
R. F. Carlton[§]

[Abstract of *Nucl. Sci. Eng.* 85, 261 (1983)]

The neutron total cross sections of ^{249}Bk and ^{249}Cf have been measured from 0.03 to 100 eV using the Oak Ridge Electron Linear Accelerator as a source of pulsed neutrons. The 1.6-mm-diam cylindrical transmission samples initially contained up to 5.3 mg of 98% ^{249}Bk and 2%

^{249}Cf; 4.5 yr later, when the final measurements were made, the composition of the samples had become 2.5% ^{249}Bk, 96.9% ^{249}Cf, and 0.6% ^{245}Cm. Samples were cooled with liquid nitrogen to reduce Doppler broadening. Thirty-nine resonances were identified in ^{249}Bk and analyzed using a single-level Breit-Wigner formalism. Fifty-five resonances were identified in ^{249}Cf and analyzed using an R-matrix multilevel formalism. The resonance parameters obtained have been used to determine the average level spacings and the s-wave neutron and fission strength functions. Where possible, bound-level parameters were derived to fit the thermal neutron total cross-section data.

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[*] Research sponsored by U.S. DOE Division of Nuclear Sciences.

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1.22

MEASUREMENT OF THE ^{232}Th(n,f) SUBTHRESHOLD AND NEAR-SUBTHRESHOLD CROSS SECTION[*]

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J. H. Todd[†] J. T. Yang[‡]
G. F. Auchampaugh[§]

[Abstract of *Phys. Rev. C* 28(4), 1635 (1983)]

A measurement of the ^{232}Th(n,f) cross section for incident neutron energies between 100 eV and 1.6 MeV has been performed at the Oak Ridge Electron Linear Accelerator. The weak subthreshold fission cross section found in this measurement confirms the model of a low first barrier in the triple-humped fission barrier which has been theoretically predicted for the (^{232}Th + n) system. However, the appearance of a series of plateaus in the near-threshold fission cross section region presents a challenge to current barrier calculations in the ^{233}Th compound nucleus.

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[*] Research sponsored by U.S. DOE Division of Reactor Research and Technology.

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1.23

HIGH-RESOLUTION MEASUREMENTS AND R-MATRIX ANALYSIS OF THE TOTAL AND FISSION CROSS SECTIONS OF ^{237}Np + n FROM 1 TO 600 eV[*]

G. F. Auchampaugh[†] M. S. Moore[†]
J. D. Moses[†] R. O. Nelson[†]
C. E. Olsen[†] R. C. Extermann[†]
N. W. Hill[‡] J. A. Harvey

(Abstract of Los Alamos Report LA-9756-MS, May 1983)

High-resolution measurements of the total and fission cross sections of ^{237}Np + n have been made using the pulsed-neutron facilities at the Oak Ridge Electron Linear Accelerator and at the Los Alamos Meson Physics Facility. The samples were cooled to liquid-nitrogen temperature. This report presents the total and fission cross sections from 1 to 600 eV, as well as the parameters obtained from an R-matrix fit of these data.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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1.24

NEUTRON FISSION CROSS SECTIONS OF ^{239}Pu AND ^{240}Pu RELATIVE TO ^{235}U[*]

L. W. Weston J. H. Todd[†]

[Abstract of *Nucl. Sci. Eng.* 84, 248 (1983)]

The ratios of the neutron fission cross sections $\sigma_f(^{240}\mathrm{Pu})/\sigma_f(^{239}\mathrm{Pu})$, $\sigma_f(^{240}\mathrm{Pu})/\sigma_f(^{235}\mathrm{U})$, and $\sigma_f(^{239}\mathrm{Pu})/\sigma_f(^{235}\mathrm{U})$ have been measured simultaneously with a multiplate ionization fission chamber using the Oak Ridge Electron Linear Accelerator as a neutron source over the neutron energy range from 5 keV to 20 MeV. The ^{240}Pu ratio data are in overall agreement with ENDF/B-V with exceptions in relatively narrow neutron energy regions. Below 150 keV and from 10 to 20 MeV, the present ^{239}Pu/^{235}U fission ratios indicate significant discrepancies when compared to ENDF/B-V. These ratios are important for thermal and fast reactor applications.

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[*] Research sponsored by U.S. DOE Office of Reactor Research and Technology.

[†] Instrumentation and Controls Division.

1.25

MEASUREMENT OF THE ^{241}Am NEUTRON FISSION CROSS SECTION[*]

J. W. T. Dabbs C. H. Johnson[†]
C. E. Bemis, Jr.[†]

[Abstract of *Nucl. Sci. Eng.* 83, 22 (1983)]

The fission cross section of ^{241}Am has been measured from 0.02 eV to 20 MeV using time-of-flight techniques at the Oak Ridge Electron Linear Accelerator. A "honeycomb" fission ionization chamber that contained six deposits totaling 1.43 mg of ^{241}Am, six deposits totaling 116 mg of ^{235}U, and a single deposit of ^{252}Cf, which served as a monitor for the chamber performance, was used. The ^{235}U fission served as the cross-section standard for energies above 101 keV while ^{6}Li(n,α), normalized to ^{235}U fission in the 7.8- to 11.0-eV interval, served as a shape standard below 101 keV. Approximately 700 h of data were obtained at a flight path distance of 9.1 m, primarily with 40-ns bursts. Because the fission cross section of ^{241}Am is very small in the midrange of neutron energies, particular attention was paid to correction of backgrounds, particularly inscattered neutron-induced events. The fission resonance integral was found to be 14.1 ± 0.9/ b.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

[†] Physics Division.

1.26

MEASUREMENT OF THE ^{242m}Am NEUTRON FISSION CROSS SECTION[*]

J. W. T. Dabbs C. E. Bemis, Jr.[†]
S. Raman[†]

[Abstract of *Nucl. Sci. Eng.* 84, 1 (1983)]

The fission cross section of ^{242m}Am has been measured from 0.005 eV to 20 MeV using time-of-flight techniques at the Oak Ridge Electron Linear Accelerator. A hemispherical plate fission ionization chamber with five pairs of plates contained three deposits totaling 507 μg of ^{242m}Am, one deposit of 168 μg ^{235}U, and a "weightless" deposit of ^{252}Cf, which served as a monitor of chamber performance. The fission of ^{235}U served as the cross-section standard for energies above 101 keV while ^{6}Li(n,α), normalized to ^{235}U fission in the 7.8- to 11.0-eV interval, served as a shape standard below 101 keV. Approximately 360 h of data were obtained at a flight path distance of 9.1 m, primarily with 40-ns bursts. Particular attention was paid to correction of backgrounds, especially inscattered-neutron-induced events. The fission resonance integral was found to be 1800 ± 65/ b.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

[†] Physics Division.

1.27

FISSION CROSS SECTION MEASUREMENTS OF ^{244}Cm, ^{246}Cm AND ^{243}Cm[+][*]

C. R. S. Stopa[†] H. T. Maguire, Jr.[‡]
D. R. Harris[†] R. C. Block[†]
R. E. Slovacek[‡] J. W. T. Dabbs
R. Hoff[§] R. Lougheed[§]

[Abstract of paper presented at ANS Topical Meeting on Advances in Reactor Physics and Core Thermal Hydraulics, Kiamesha Lake, NY, September 22-24, 1982; Proc. NUREG/CP-0034, Vol. 1, p. 1090 (1982)]

The RINS (Rensselaer Intense Neutron Spectrometer) system, which includes a 75-ton lead slowing-down-time spectrometer and the RPI

100-MeV electron linac, has been used to measure the neutron-induced fission cross sections of ^{244}Cm, ^{246}Cm and ^{248}Cm. These isotopes have either large spontaneous fission background (e.g., ^{248}Cm) or large alpha decay rates (e.g., ^{244}Cm), and it required the high neutron intensity of the RINS system to carry out these measurements. Preliminary measurements of ^{244}Cm, ^{246}Cm and ^{248}Cm have been reported previously, and this paper includes the earlier results, combined with the results of a recent measurement in which all three isotopes were measured simultaneously. The fission chamber consists of five pairs of hemispherical electrodes contained in 2 atm of methane, and for the latest measurements the electrodes were coated with ^{244}Cm (5.2 μg), ^{246}Cm (17 μg), ^{248}Cm (35 μg), ^{235}U and ^{252}Cf. The ^{235}U chamber was used for normalization, and the ^{252}Cf chamber monitored any effects caused at early slowing-down times by the linac gamma flash or by RF pickup from the pulsing of the accelerator.

These measurements span the energy range from 0.1 eV to 100 keV. The data below ~20 eV are the first obtained in this energy range, and the data above ~20 eV complement the nuclear explosion time-of-flight measurements. Low-energy resonances have been resolved at 7.7, 17, 23 and 35 eV in ^{244}Cm; 4.3 and 15 eV in ^{246}Cm; and 7.3, 27 and 76 eV in ^{248}Cm. Parameters will be determined for these resonances.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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1.28

FAST NEUTRON INELASTIC SCATTERING FROM ^{56,57}Fe*

J. K. Dickens

[Abstract of *Bull. Am. Phys. Soc.* 27(7), 716 (1982)]

ORELA produced neutrons were used to measure gamma-ray production cross sections due to neutron reactions with ^{56,57}Fe for incident neutron energies $0.16 \leq E_n \leq 40$ MeV. Data reduction for $^{57}\mathrm{Fe}(n,n'\gamma)$ are compared with compound-nucleus calculations. The agreement is reasonable for $E_n < 3$ MeV.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

1.29

NEUTRON-INDUCED GAMMA-RAY PRODUCTION IN ^{57}Fe FOR INCIDENT-NEUTRON ENERGIES BETWEEN 0.16 AND 21 MeV*

Z. W. Bell[†] J. K. Dickens
D. C. Larson J. H. Todd[‡]

[Abstract of *Nucl. Sci. Eng.* 84, 12 (1983)]

Interactions of neutrons with the iron isotope ^{57}Fe have been studied by measuring gamma-ray production cross sections for incident-neutron energies between 0.16 and 21 MeV. Neutrons produced by the Oak Ridge Electron Linear Accelerator impinged on a metallic iron sample enriched to 93% in the isotope ^{57}Fe. The resulting gamma radiation was detected using a 100-cm^3 Ge(Li) detector placed at 125 deg with respect to the neutron beam line. A complete description of the experiment is given. Absolute gamma-ray production cross sections were measured for gamma rays corresponding to the $^{57}\mathrm{Fe}(n,n'\gamma)^{57}\mathrm{Fe}$, $^{57}\mathrm{Fe}(n,\gamma)^{58}\mathrm{Fe}$, $^{57}\mathrm{Fe}(n,\alpha)^{54}\mathrm{Cr}$, $^{57}\mathrm{Fe}(n,2n)^{56}\mathrm{Fe}$, and $^{57}\mathrm{Fe}(n,p)^{57}\mathrm{Mn}$ reactions. The cross section for the $^{57}\mathrm{Fe}(n,2n)^{56}\mathrm{Fe}$ reaction exceeds 1 b for E_n ~15 MeV, and the cross section for the $^{57}\mathrm{Fe}(n,p)^{57}\mathrm{Mn}$ reaction exceeds 0.2 b for E_n ~9 MeV. A new excited state is postulated for ^{57}Mn to account for observed data. Several new transitions are reported for decay of levels in ^{57}Fe. Measured cross sections are compared with data obtained from the current ENDF/B evaluation.

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[*] Research sponsored by U.S. DOE Division of Basic Energy Sciences.

[†] UCC-ND Computer Sciences Division.

[‡] Instrumentation and Controls Division.

1.30

GAMMA-RAY DECAY OF LEVELS IN ^{63}Cu AND ^{65}Cu[*]

J. K. Dickens

[Abstract of *Nucl. Phys.* A401, 189 (1983)]

Gamma-ray decay of levels in the stable copper isotopes ^{63}Cu and ^{65}Cu has been studied using ^{63,65}Cu($n,n'\gamma$) reactions for incident neutron energies between threshold and 6 MeV. Of the 257 γ-rays or γ-ray groups observed for neutron interactions with ^{63}Cu, 137 have been placed or tentatively placed among 88 levels in ^{63}Cu up to an excitation energy of 5.9 MeV. Similarly, of 335 γ-rays or γ-ray groups observed for neutron interactions with ^{65}Cu, 127 have been placed among 100 levels in ^{65}Cu up to an excitation energy of 5.8 MeV, including new decay data for >70 excited states of ^{65}Cu.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

1.31

GAMMA RAY PRODUCTION DUE TO NEUTRON INTERACTIONS WITH COPPER FOR NEUTRON ENERGIES BETWEEN 0.7 AND 10.5 MeV[*]

G. G. Slaughter[†] **J. K. Dickens**

[Abstract of *Nucl. Sci. Eng.* 84, 395 (1983)]

Differential cross sections for 22 gamma rays produced by neutron interactions with elemental copper having energies, E_γ, between 0.36 and 2.5 MeV have been measured for neutron energies, E_n, between 0.7 and 10.5 MeV for $\theta_\gamma = 90°$ using a Ge(Li) detector system. The present data are compared with previously reported measurements; agreement with earlier reported data is generally good for $E_n < 3$ MeV and generally poor for $E_n > 4$ MeV.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

[†] Physics Division.

1.32

CROSS SECTIONS FOR THE Mo(n,xn) REACTIONS BETWEEN 3 AND 21 MeV[*]

Z. W. Bell[†]

(Abstract of ORNL/TM-8863, October 1983)

Differential cross sections for Mo(n,xn) reactions have been measured for incident neutron energies between 3 and 21 MeV and for secondary neutron energies between 2 and 21 MeV. The data are compared with current ENDF/B evaluated data and with experimental data of two recent measurements. Discrepancies with evaluation for E_n between 5 and 9 MeV are discussed but not resolved. The present data agree reasonably well with evaluation for $E_n > 10$ MeV and with previous experimental data for $E_n = 4$ MeV.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

[†] UCC-ND Computer Sciences Division.

1.33

NEUTRON SCATTERING FROM Os ISOTOPES AT 60 keV AND Re/Os NUCLEOCHRONOLOGY[*]

R. L. Hershberger[†] **R. L. Macklin**
M. Balakrishnan[†] **N. W. Hill[‡]**
M. T. McEllistrem[†]

[Abstract of *Phys. Rev. C* 28(6), 2249 (1983)]

Neutron elastic and inelastic scattering cross sections have been measured for 60.5 keV neutrons incident on ^{187,188}Os. For ^{187}Os the cross section for elastic scattering is 11 b and for inelastic scattering to the 9.75-keV level it is 1.13 b. These results and other scattering properties are represented in phase shift and scattering potential analyses, which then allow the prediction of neutron capture by ^{187}Os nuclei in the 9.75-keV and ground levels. Capture rates thus provided are used in the Re/Os nucleochronology, and lead to a long galactic age, about 10 to 20 Gyr.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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[‡] Instrumentation and Controls Division.

1.34

^{187}Os(n,n') INELASTIC CROSS SECTION AT 34 keV*

R. L. Macklin R. R. Winters[†]
N. W. Hill[‡] J. A. Harvey

[Abstract of *Astrophysical Journal* 274, 408 (1983)]

A measurement of the ^{187}Os inelastic neutron cross section to the $3/2^-$, 9.75-keV excited state with 34 ± 2 keV incident neutrons gives 1.5 ± 0.2 barns. Pulsed neutron time of flight and a short anisotropic iron-aluminum filter allowed separation of the inelastic yield from the $1/2^-$ ground-state elastic yield at 24 keV. The influence of the result on *r*-process galactic age calculations via the Re-Os decay chronometer is discussed, and the need for further theoretical calculations is emphasized.

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*Research sponsored by U.S. DOE Division of Nuclear Sciences.

[†] Denison University, Granville, OH.

[‡] Instrumentation and Controls Division.

1.35

GAMMA-RAY TRANSITIONS AMONG LEVELS OF ^{206}Pb*

J. K. Dickens

[Abstract of *Phy. Rev. C* 28(2), 916 (1983)]

A study of γ-ray data produced by neutron inelastic scattering from a lead sample enriched in the isotope ^{206}Pb has resulted in placements of 106 γ rays as transitions among 88 known or postulated levels of the ^{206}Pb level structure.

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*Research sponsored by U.S. DOE Office of Basic Energy Sciences.

Cross-Section Analyses, Evaluations, and Reviews

1.36

EXPERIMENTAL AND CALCULATIONAL ANALYSES OF ACTINIDE SAMPLES IRRADIATED IN EBR-II*

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R. L. Walker[‡] S. Raman[§]
P. H. Stelson[§]

(Abstract of ORNL-5791, October 1982)

Higher actinides influence the characteristics of spent and recycled fuel and dominate the long-term hazards of the reactor waste. Reactor irradiation experiments provide useful benchmarks for testing the evaluated nuclear data for these actinides. During 1967-1970, several actinide samples were irradiated in the Idaho EBR-II fast reactor. These samples have now been analyzed, employing mass and alpha spectometry, to determine the heavy element products. A simple spherical model for the EBR-II core and a recent version of the ORIGEN code with ENDF/B-V data were employed to calculate the exposure products. A detailed comparison between the experimental and calculated results has been made. For samples irradiated at locations near the core center, agreement within 10% was obtained for the major isotopes and their first daughters, and within 20% for the nuclides up the chain. A sensitivity analysis showed that the assumed flux should be increased by 10%. The lessons learned from the present study were incorporated into the planning of a future irradiation study to be carried out in the UK Prototype Fast Reactor at Dounreay.

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*Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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[‡] Analytical Chemistry Division.

[§] Physics Division.

1.37

RESONANCE PARAMETERS OF ^{60}Ni + *n* FROM MEASUREMENTS OF TRANSMISSION AND CAPTURE YIELDS FROM 1 TO 450 keV[*]

C. M. Perey J. A. Harvey
R. L. Macklin R. R. Winters[†]
F. G. Perey

[Abstract of ORNL-5893, November 1982; also *Phys. Rev. C* 27(6), 2556 (1983)]

High-resolution transmission and capture measurements of ^{60}Ni-enriched targets have been made from a few eV to 1800 keV in transmission and from 2.5 keV to 5 MeV in capture. The transmission data from 1 to 452 keV were analyzed with a multilevel $\tilde{R}$-matrix code which uses the Bayes' theorem for the fitting process. This code provides the energies and neutron widths of the resonances inside the 1- to 452-keV region as well as a possible parameterization for outside resonances to describe the smooth cross section in this region. The capture data were analyzed from 2.5 to 452 keV with a least-squares fitting code using the Breit-Wigner formula. Average parameters for the 30 observed s-wave resonances were deduced. The average level spacing, D_o, was found to be equal to 15.2 ± 1.5 keV; the strength function, S_o, equal to $(2.2 \pm 0.6) \times 10^{-4}$; and the average radiation width, Γ_γ, equal to 1.30 ± 0.07 eV. The staircase plot of the reduced level widths and the plot of the Lorentz-weighted strength function averaged over various energy intervals show possible evidence for doorway states. The level densities calculated with the Fermi-gas model for $\ell = 0$ and for $\ell > 0$ resonances were compared with the cumulative number of observed resonances, but the analysis is not conclusive. The correlation coefficient ρ between Γ_n^o and Γ_γ is equal to 0.53 ± 0.18. The average capture cross section as a function of the neutron incident energy is compared to the tail of the giant electric dipole resonance prediction.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

[†] Denison University, Granville, Ohio.

1.38

RESOLVED RESONANCE PARAMETERS FOR ^{238}U FROM 4 TO 6 keV[*]

D. K. Olsen P. S. Meszaros[†]

[Abstract of *Nucl. Sci. Eng.* 83, 174 (1983)]

Neutron widths for 145 resonances from 4 to 6 keV are reported from a least-squares shape analysis of the ORELA 150-m, 4-sample ^{238}U transmission data. The resultant s-wave strength function from 4 to 6 keV is found to be substantially smaller than that from 0 to 4 keV.

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[*] Research sponsored by U.S. DOE Office of Reactor Research and Technology.

[†] UCC-ND Computer Sciences Division.

1.39

OBSERVED ℓ-DEPENDENCE OF NEUTRON OMP REAL WELL DEPTHS FOR ^{30}Si AND ^{34}S[*]

C. H. Johnson[†] J. A. Harvey
R. F. Carlton[‡]

[Abstract of *Bull. Am. Phys. Soc.* 28(4), 648 (1983)]

From the R-matrix parameters required to fit high resolution transmission data for 0.0 to 1.5 MeV neutrons on ^{30}Si and ^{34}S we have deduced average s- and p-wave scattering functions in the same manner as done previously for ^{32}S. When we fit these averages using a spherical optical model potential, we find, within the uncertainties of about ± 1 MeV, the same real well depths for ^{30}Si and ^{34}S as obtained previously for ^{32}S, namely 61.5 MeV for p-waves and 51.5 MeV for s-waves. (The real well had $r_o = 1.21$ f and $a = 0.66$ f.) For ^{32}S this ℓ-dependence has been explained in terms of deformations. It is reasonable that the ℓ-dependence for ^{30}Si and ^{34}S can also be attributed to deformations.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

[†] Physics Division.

[‡] Middle Tennessee State University, Murfreesboro, TN.

1.40

PROBLEMS AND PROGRESS REGARDING RESONANCE PARAMETERIZATION OF ^{235}U AND ^{239}Pu FOR ENDF/B[*]

M. S. Moore[†] G. de Saussure
G. R. Smith[‡]

(Abstract of a paper presented at Symposium on Uranium and Plutonium Isotope Resonance Parameters, Vienna, Austria, September 28 - October 2, 1981)

The procedures used to obtain the resolved and unresolved resonance parameterization of ^{235}U and ^{239}Pu contained in the U.S. Evaluated Nuclear Data File ENDF/B-V are reviewed. For ^{235}U, recommendations are made to improve the representation by including information on resonance spins and fission-channel vector orientations, and some preliminary results are presented. We review evidence that it is the fission channels rather than the spins of the resonances that lead to differences in fission mass distributions, the number of neutrons emitted per fission, and fission kinetic energies. The improved parameterization may thus have physics content that will prove of interest in future applications.

[*] Research sponsored by U.S. DOE Division of Reactor Research and Technology.

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1.41

IMPLEMENTATION OF AN ADVANCED PAIRING CORRECTION FOR PARTICLE-HOLE STATE DENSITIES IN PRECOMPOUND NUCLEAR REACTION THEORY[*]

C. Y. Fu

(Abstract of *Nucl. Sci. Eng.*, in press)

An advanced pairing correction for an existing formula of particle-hole state densities, needed in calculation of cross sections with the precompound nuclear reaction theory, is examined. The Pauli correction is derived to be consistent with this pairing correction. The accuracy of the pairing correction plus the Pauli correction is shown to be sufficient for applied calculations. Numerical solutions of the pairing equations, needed for generating the corrections, have been carried out. The relevant numerical results are presented as simple functions of the excitation energy and the exciton number. A relationship between the pairing correction for particle-hole state densities and the pairing correction for the total state densities in the closed-form formulation is developed. Utilization of the existing level-density parameter and data for deducing parameters for the particle-hole state densities is shown.

[*] Research sponsored by U.S. DOE Division of Basic Energy Sciences.

1.42

PAIRING CORRECTION FOR PARTICLE-HOLE STATE DENSITIES[*]

C. Y. Fu

(Abstract of paper presented at IAEA Advisory Group Meeting on Basic and Applied Problems of Nuclear Level Densities, Upton, New York, April 11-15, 1983)

The pairing correction proposed by Ignatyuk and Sokolov for particle-hole state densities has been examined. It has been found that the accuracy of the correction is sufficient for practical applications only if the system is in its normal state $(\Delta = 0)$. In the superfluid state $(\Delta \neq 0)$, a consistent pairing-Pauli correction is developed here for improved accuracy. Practical implementations of the pairing correction are given and further developments are outlined.

[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

1.43

COMMENT ON "DETERMINATION OF GAMMA-RAY ENERGIES AND ABUNDANCES OF ^{229}Th"[*]

J. K. Dickens

[Abstract of *Phys. Rev. C* 28, 1404 (1983)]

It is shown that the absolute normalization of γ-ray yields (I_γ) for transitions among levels in

^{225}Ra following α decay of ^{229}Th reported by Rattan *et al.* should be increased by at least 22%. Disagreements of reported values of I_γ with those in a recent report are discussed but not resolved.

[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

1.44

ELECTRON SPECTRA FROM DECAY OF FISSION PRODUCTS[*]

J. K. Dickens

(Abstract of ORNL/TM-8255, September 1982)

Electron spectra following decay of individual fission products (72 ≤ A ≤ 162) are obtained from the nuclear data given in the compilation using a listed and documented computer subroutine. Data are given for more than 500 radionuclides created during or after fission. The data include transition energies, absolute intensities, and shape parameters when known. An "average" beta-ray energy is given for fission products lacking experimental information on transition energies and intensities. For fission products having partial or incomplete decay information, the available data are utilized to provide best estimates of otherwise unknown decay schemes. This compilation is completely referenced and includes data available in the reviewed literature up to January 1982.

[*] Research sponsored by U.S. DOE Division of Basic Energy Sciences.

1.45

s-PROCESS STUDIES IN THE LIGHT OF NEW EXPERIMENTAL CROSS SECTIONS: DISTRIBUTION OF NEUTRON FLUENCES AND *r*-PROCESS RESIDUALS[*]

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K. Wisshak[†] D. D. Clayton[‡]
R. L. Macklin R. A. Ward[§]

[Abstract of *Astrophysical J.* 257, 821 (1982)]

A best set of neutron-capture cross sections has been evaluated for the most important *s*-process isotopes. With this data base, *s*-process studies have been carried out using the traditional model which assumes a steady neutron flux and an exponential distribution of neutron irradiations. The calculated σN curve is in excellent agreement with the empirical σN-values of pure *s*-process nuclei. Simultaneously, good agreement is found between the difference of solar and *s*-process abundances and the abundances of pure *r*-process nuclei. We also discuss the abundance pattern of the iron group elements where our *s*-process results complement the abundances obtained from explosive nuclear burning. The results obtained from the traditional *s*-process model such as seed abundances, mean neutron irradiations, or neutron densities are compared to recent stellar model calculations which assume the He-burning shells of red giant stars as the site for the *s*-process.

[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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[§] Max-Planck-Institut für Physik und Astrophysik, München.

1.46

NEW DEVELOPMENTS IN THE UNRESOLVED RANGE[*]

R. B. Perez G. de Saussure

[Abstract of paper presented at the Specialists' Workshop on ^{238}U Capture in Fast Reactors, Teton Village, Wyoming, June 22-24, 1982; Proc. 2B (1982)]

Considerable amounts of effort have gone into improving processing methods in the unresolved region but substantially less into validating them as a representation of the ^{238}U(n,γ) cross section in the unresolved region. The unresolved resonance-region methodology endeavors to: (1) reconstruct the infinitely diluted cross sections, and (2) provide a formalism to calculate self-shielding factors as a function of temperature and dilution.

The purpose of this paper is to examine the sensitivity of self-shielding factor calculations in the unresolved resonance region to both average resonance parameters and calculation methods. We have observed that: (a) presently available average resonance parameters are not fully consistent for self-shielding factor calculations in the unresolved region, and (b) large uncertainties arise from statistical sampling errors in the Monte Carlo method utilized in the unresolved resonance region. These results lead to the conclusion that whenever resonance self-shielding is important, one should parametrize the gross features of the cross section so that resolved resonance region methods could be utilized, while treating only the smaller resonances by statistical methods or by a File 3 smooth contribution approach. In summary we recommend the extension of the ^{238}U resolved resonance region up to roughly 10 keV.

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[*] Research sponsored by U.S. DOE Division of Reactor Research and Technology.

1.47

UNCERTAINTIES IN THE ^{238}U RESOLVED RESONANCE PARAMETERS AND THEIR IMPACT ON CALCULATED GROUP CONSTANTS[*]

G. de Saussure R. Q. Wright[†]
R. B. Perez

[Abstract of paper presented at the Second Jackson Hole Colloquium on Fast Reactor Physics: The Doppler Effect in LMFBRs, Teton Village, Wyoming, June 27-29, 1983; Proc. Session III, No. 3 (1983)]

In assessing the contribution of the uncertainties in a data set to the uncertainty in a computed performance parameter (such as capture to fission ratio in a benchmark, or Doppler coefficient of reactivity), it is required to assess the uncertainty in the pertinent group constants due to uncertainty in the basic data.

In this presentation we will review the data base for the ENDF/B-V evaluation of the ^{238}U resolved resonance parameters and show how the analysis of the data base leads to the estimated systematic uncertainties in the evaluated parameters. We will then show how these systematic uncertainties propagate to uncertainties in Bondarenko-type group constants as a function of dilution and temperature. The impact on benchmarks is discussed in the presentation of R. Q. Wright.

We will also compare the ENDF/B-V ^{238}U resolved resonance parameters with those of two recent independent evaluations (JENDL-2 and Moxon and Sowerby 1982). The comparison shows that the very different approaches used in the three evaluations lead to very consistent average data.

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[*] Research sponsored by U.S. DOE Division of Reactor Research and Technology.

[†] UCC-ND Computer Sciences Division.

1.48

IMPACT OF UNCERTAINTIES IN ^{238}U RESONANCE PARAMETERS ON PERFORMANCE PARAMETERS OF THERMAL LATTICES[*]

R. Q. Wright[†] G. de Saussure
R. B. Perez

[Abstract of *Trans. Am. Nucl. Soc.* 45, 701 (1983)]

The calculated and measured values of integral parameters may be considered discrepant if their differences are significantly greater than the combined uncertainties assigned to the integral experiment, the calculational methods, and the evaluated differential data. This paper presents an assessment of the uncertainties in the calculated values of performance parameters of selected uranium metal and uranium oxide lattices due to uncertainties in ENDF/B-V data, particularly the ^{238}U resolved resonance parameters.

ENDF/B-V provides ^{238}U resolved resonance parameter covariance files to describe the estimated uncertainties in the evaluated data, but these covariance data have not yet been applied in thermal reactor data testing. One difficulty in using resonance parameter uncertainties has been the lack of an adequate methodology to derive resonance parameter sensitivities, particularly where self-shielding effects are important.

Two kinds of uncertainties are assigned to the resonance parameters: statistical uncertainties, which are uncorrelated from one level to the next, and systematic uncertainties correlated over resolved resonances of the energy range 1 to 4000 eV. The contribution of the systematic uncertainties dominates and, therefore, was the only contribution considered in the present work.

The uncertainties in k_{eff}, ρ^{28}, δ^{25}, δ^{28}, and CR of thermal lattices due to systematic uncertainties in the ^{238}U resolved resonance parameters were obtained by recomputing the group constants for several values of the ^{238}U resolved resonance parameters corresponding to the different types of systematic uncertainties.

The uranium metal lattice TRX-1 and the uranium oxide lattice BAPL-1 were selected for this study because they have been widely used in thermal data testing. These lattices have ^{238}U dilution, σ_0, of 21.3 and 45.0 b, respectively.

Calculational methods uncertainties are difficult to assess. Ignoring the methods uncertainties, it can be concluded that (a) the measured and calculated values of the TRX-1 and BAPL-1 parameters are reasonably consistent when uncertainties in the differential data and integral measurements are considered, and (b) the uncertainties due to the ^{238}U resolved resonance parameters are the most significant contribution to the uncertainties in the calculated values of ρ^{28} and CR for thermal lattices.

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[*] Research sponsored by Nuclear Power Division of the Electric Power Research Institute (EPRI).

[f] UCC-ND Computer Sciences Division.

1.49

IMPACT OF UNCERTAINTIES IN ^{238}U RESONANCE CAPTURE CROSS SECTIONS ON BENCHMARK PERFORMANCE PARAMETERS[*]

R. Q. Wright[f] G. de Saussure
R. B. Perez

[Abstract of paper presented at the Second Jackson Hole Colloquium on Fast Reactor Physics: The Doppler Effect in LMFBRs, Teton Village, Wyoming, June 27-29, 1983; Proc. Session IV, No. 5 (1983)]

Calculated uncertainties in CSEWG fast reactor benchmarks using uranium and plutonium evaluations from ENDF/B-V are a major concern to the fast reactor community. As an example, the performance parameters for the plutonium oxide fueled ZPR-6/7 and the uranium oxide fueled ZPR-6/6A benchmarks are reviewed.

In a companion paper, de Saussure et al. describe uncertainties in the ^{238}U Bondarenko-type group constants, as a function of dilution and temperature, prepared from the ENDF/B-V ^{238}U evaluation.[1] Sensitivity calculations were used to investigate the effect of changes in the group constants on the benchmark performance parameters. In this presentation, the impact of the uncertainties in the ^{238}U capture cross sections on ZPR-6/7 and ZPR-6/6A eigenvalues and central reaction rate ratios are discussed. Of special interest are performance parameter uncertainties resulting from uncertainties in resolved resonance Γ_n and Γ_γ and in the unresolved resonance range. The impact of uncertainties in ^{238}U capture will be compared to the impact due to uncertainties in ^{239}Pu fission for the ZPR-6/7 eigenvalue and ^{238}U capture/^{239}Pu fission reaction ratio at the center of the one-dimensional spherical model of the assembly.

Revision 2 to the ENDF/B-V ^{239}Pu has been proposed.[2] The impact of the proposed evaluation on performance parameters of Pu-fueled benchmark assemblies are discussed.

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[*] Research sponsored by U.S. DOE Division of Reactor Research and Technology.

[f] UCC-ND Computer Sciences Division.

1. G. de Saussure, R. Q. Wright, and R. B. Perez, paper 1.46, this report.
2. E. D. Arthur, *Los Alamos Evaluation of ^{239}Pu for Revision 2 of ENDF/B-V*, LANL, January 24, 1983.

1.50

FAST REACTOR DATA TESTING OF ENDF/B-V AT ORNL[*]

R. Q. Wright[f] W. E. Ford, III[f]
J. L. Lucius[f] C. C. Webster[f]
J. H. Marable

[Abstract of paper presented at ANS Topical Meeting on Advances in Reactor Physics and Core Thermal Hydraulics, Kiamesha Lake, NY, September 22-24, 1982; Proc. NUREG/CP-0034, Vol. 2, p. 1135 (1982)]

Data from the ENDF/B-V processed multigroup cross-section libraries VITAMIN-E and

FORSS-V were used in the calculation of twelve CSEWG fast reactor benchmarks. Results obtained include the eigenvalues, central reaction rate ratios, and central reactivity worths. Conclusions and recommendations based on the trends in these results are given. Finally, the ORNL results are compared with those obtained by other data testers.

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[*] Research sponsored by U.S. Department of Energy.

[†] UCC-ND Computer Sciences Division.

1.51

BENCHMARK DATA TESTING OF ENDF/B-V[*]

Edited by

C. R. Weisbin   R. D. McKnight[†]
J. Hardy, Jr.[‡]   R. W. Roussin
R. E. Schenter[§]   B. A. Magurno[¶]

[Abstract of BNL-NCS-31531 (ENDF-311), August 1982]

The testing of Cross Section Evaluation Working Group (CSEWG) data is primarily intended to assess the adequacy of ENDF/B nuclear data for use in nuclear design and applications. The purpose of this report is to describe the results of the benchmark testing of ENDF/B-V and to identify areas of basic nuclear data and computational methods and integral experiments that may require additional research. The benchmark testing is classified according to five major applications: (1) fast reactor design, (2) thermal reactor design, (3) radiation shielding design, (4) fission product and actinide analyses, and (5) dosimeter response analyses. In each case the analyses of pertinent integral experiments are presented and the current limitations in the data-testing process are discussed. Finally, areas of agreement and disagreement are pointed out, and recommendations for future investigations are given.

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[*] Research sponsored by U.S. Department of Energy.

[†] Argonne National Laboratory, Argonne, IL.

[‡] Bettis Atomic Power Laboratory, West Mifflin, PA.

[§] Hanford Engineering Development Laboratory, Richland, WA.

[¶] Brookhaven National Laboratory, Upton, NY.

1.52

ORELA CONTRIBUTION TO THORIUM CYCLE NUCLEAR DATA[*]

D. K. Olsen

(Abstract of paper presented at the U.S.—Japan Joint Seminar on the Thorium Fuel Cycle, Nara, Japan, October 18-22, 1982)

The measurements of direct importance to the ^{232}Th/^{233}U fuel cycle using neutrons from the Oak Ridge Linear Accelerator facility are gathered together and discussed. These measurements were done in response to specific data discrepancies, as part of generic programs, and for basic fission physics studies. In particular, completed transmission and capture work on ^{232}Th has yielded the most accurate parameters for the first four s-wave resonances; the largest average capture width, 25.2 meV; and the largest s-wave strength function of recent measurements. These results allow improved agreement between differential and integral capture rates. Moreover, the ORNL ^{252}Cf $\bar{\nu}$ measurement of unprecedented accuracy and ^{233}U $\bar{\nu}$ ratio measurement give a ^{233}U prompt $\bar{\nu}$ (thermal) of 2.490 ± 0.009 neutrons/fission. This result allows a much more satisfactory understanding of the ^{233}U 2200-m/s constants. In addition, a ^{232}Th γ-ray production measurement provides needed cross sections for shielding, and important data for both application and fission physics were obtained from ^{232}Th fission and both ^{231}Pa and ^{234}U fission and total cross section measurements. Data requirements and discrepancies suggested from this work are discussed.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

1.53

THE NUCLEAR DATA OF THE MAJOR ACTINIDE FUEL MATERIALS[*]

W. P. Poenitz[†]   G. de Saussure

(Abstract of chapter in *Cross-Section Data for Nuclear Reactor Analyses*, Progress in Nuclear Energy series, Pergamon Press, Oxford, in press)

Nuclear data for the major actinides (^{232}Th, ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, and ^{242}Pu) are reviewed with respect to their application in the optimization of fuel cycles and core designs for thermal and fast breeder reactors. The most important measurements are reviewed and the consistency and completeness of contemporary evaluations (ENDF-V, JENDL-2, KEDAK, SOKRATOR, etc.) are compared. The impact of uncertainties or discrepancies in the data on neutronic calculations is assessed.

[*] Research sponsored by U.S. Department of Energy.

[†] Argonne National Laboratory, Argonne, IL.

1.54

MICROSCOPIC BETA AND GAMMA DATA FOR DECAY HEAT NEEDS[*]

J. K. Dickens

(Abstract of paper presented at the OECD/NEA Nuclear Data Committee Specialists Meeting on Yields and Decay Data, Fission Product Nuclides, Brookhaven National Laboratory, Upton, New York, October 23-27, 1983)

Microscopic beta and gamma data for decay heat needs are defined as absolute intensity spectral distributions of beta and gamma rays following radioactive decay of radionuclides created by, or following, the fission process. Four well-known evaluated data files, namely the U.S. ENDF/B-V, the U.K. UKFPDD-2, the French BDN (for fission products), and the Japanese JNDC Nuclear Data Library, are reviewed. Comments regarding the analyses of experimental data (particularly gamma-ray data) are given; the need for complete beta-ray spectral measurements is emphasized. Suggestions on goals for near-term future experimental measurements are presented.

[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

1.55

REPORT TO THE DOE NUCLEAR DATA COMMITTEE[*]

F. G. Perey

(Abstract of BNL-NCS-32614, p. 134, May 1983)

This report was prepared for the DOE Nuclear Data Committee and covers work performed at ORNL since January 1982 in areas of nuclear data of relevance to the U.S. applied nuclear energy program. The report was mostly generated through a review of abstracts of work completed to the point of being subjected to some form of publication in the open literature, formal ORNL reports, ORNL technical memoranda, progress reports, or presentation at technical conferences. As much as possible we have reproduced the complete abstract of the original publication with only minor editing. In a few cases progress reports were written specifically for this publication. The editors have selected the materials to be included in this report on the basis of perceived interests of DOE Nuclear data Committee members and cannot claim completeness.

[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

Research Techniques and Facilities

1.56

OFFICE OF BASIC ENERGY SCIENCES PROGRAM TO MEET HIGH PRIORITY NUCLEAR DATA NEEDS OF THE OFFICE OF FUSION ENERGY (1983 REVIEW)[*]

R. C. Haight[†] D. C. Larson[‡]
and Other Panel Members

(Abstract of Lawrence Livermore Laboratory Report UCID-19930, November, 1983)

This review was prepared during a coordination meeting held at Oak Ridge National Laboratory on September 28-29, 1983. Participants included research scientists working for this program, a representative from the OFE's Coordination of Magnetic Fusion Energy (MFE) Nuclear Data Needs Activities, and invited specialists.

[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

[†] Panel chairman.

[‡] Panel secretary.

1.57

USER'S GUIDE FOR BAYES: A GENERAL-PURPOSE COMPUTER CODE FOR FITTING A FUNCTIONAL FORM TO EXPERIMENTAL DATA*

N. M. Larson[†]

[Abstract of ORNL/TM-8185 (ENDF-323), August 1982]

This report is intended as a user's manual for a general-purpose computer program BAYES to solve "Bayes' equations" for updating parameter values, uncertainties, and correlations. Bayes' equations are derived from Bayes' theorem, using linearity and normality assumptions. The method of solution is described, and details are given, including problem description and solution method, FORTRAN coding, and sample input and output. A companion code LEAST, which solves the usual least-squares equations rather than Bayes' equations but which encourages non-diagonal data weighting, is also described.

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*Research sponsored by U.S. Department of Energy.

[†] UCC-ND Computer Sciences Division.

1.58

APPLICATION OF GROUP THEORY TO DATA REDUCTION*

F. G. Perey

(Abstract of ORNL-5908, September 1982)

The analysis within the framework of a theory of what was observed in experiments is essential to the testing of theories and is fundamental to physics. It is shown in this report how group theory can be used to provide a general method of data reduction whereby only the laws of a particular theory are used in the analysis of observations. This application of group theory involves introducing a group of transformations of the physical system upon which the observations were made. This group of transformations leaves invariant the entities of the theory corresponding to the observations made but transforms the entities that were not observed from what they are presumed to be in this theory into what they are not, called possibilities for what they are. This group of transformations is called the possibilities-generating group for the entities for which the observations are being reduced. Since possibilities for entities of theories so obtained are functionals of a known group of transformations, the subsequent use of these possibilities in the theories must be made consistent with the theory of representations of groups. There is a well-known invariant associated with functionals of group elements which is invariant with respect to the parametrization of this group. It is the normalized volume measure in the group manifold of the possibilities-generating group. In this report this invariant measure is called the physical probability of the possibilities since it is a probability measure which has a Borel algebra. The above proposed method of data reduction allows us to deal unambiguously with the uncertainties in entities of physical theories obtained from all of the observations made in experiments and the distinction between systematic and statistical uncertainties disappears. Concrete realizations of possibilities-generating groups are given and explanations in group theoretical terms are offered for several important intuitive notions related to probabilities.

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*Research sponsored by U.S. DOE Office of Basic Energy Sciences.

1.59

COUNTING ANTICOINCIDENCES TO REDUCE STATISTICAL UNCERTAINTY IN THE CALIBRATION OF A MULTIPLICITY DETECTOR*

R. W. Peelle R. R. Spencer

[Abstract of *Nucl. Instrum. Methods* 211, 167 (1983)]

The observation of anticoincidences reduced statistical uncertainties as well as pileup corrections in the efficiency calibration of a multiplicity detector. The efficiency of the 4π gadolinium-loaded organic scintillation detector was measured for detecting capture of neutrons scattered by the hydrogen in a second detector. In such situations the effect of background upon the counting fluctuations is reduced below the value that would occur if the average counting rate during coincidence gates were utilized. The applicable formulae were obtained by elementary methods and were verified with experimental data and with computer simulations for a broad range of detector efficiencies and background intensities. The general requirements for use of the technique are indicated.

[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

1.60

AN ANNOTATED BIBLIOGRAPHY COVERING GENERATION AND USE OF EVALUATED CROSS-SECTION UNCERTAINTY FILES[*]

R. W. Peelle T. W. Burrows[†]

[Abstract of BNL-NCS-51684 (ENDF-331), March 1983]

Literature references related to evaluated cross-section uncertainty (variance-covariance) files are listed with comments intended primarily to guide the reader toward materials of immediate interest. Papers are included that cover covariance information from individual experiments and that relate to production and use of multigroup covariance matrices. Titles are divided among several major categories. The comments by the compilers may not reflect the views of the authors of the papers cited.

[*] Research sponsored by U.S. DOE Office of Reactor Research and Technology.

[†] Brookhaven National Laboratory, Upton, NY.

1.61

NEUTRON FILTERS FOR PRODUCING MONOENERGETIC NEUTRON BEAMS[*]

J. A. Harvey N. W. Hill[†]
J. R. Harvey[‡]

[Abstract of paper presented at the International Conference on Nuclear Data for Science and Technology, Antwerp, Belgium, September 6-10, 1982; Proc. p. 856, K. H. Bockoff, Ed. (1983)]

Neutron transmission measurements have been made on high-purity, highly enriched samples of ^{58}Ni (99.9%), ^{60}Ni (99.7%), ^{64}Zn (97.9%), and ^{184}W (94.5%) to measure their neutron "windows" and to assess their potential usefulness for producing monoenergetic beams of intermediate energies from a reactor. Transmission measurements on the Los Alamos Sc filter (44.26 cm Sc and 1.0 cm Ti) have been made to determine the characteristics of the transmitted neutron beam and to measure the total cross section of Sc at the 2.0 keV minimum. When corrected for the Ti and impurities, a value of 0.35 ± 0.03 b was obtained for this minimum.

[*] Research sponsored by U.S. DOE Division of Nuclear Sciences.

[†] Instrumentation and Controls Division.

[‡] CEGB Berkeley Nuclear Laboratories, Berkeley, England.

1.62

DEVELOPMENT OF AN ATOM BUNCHER[*]

G. S. Hurst[†] M. G. Payne[†]
R. C. Phillips[†] J. W. T. Dabbs
B. E. Lehmann[‡]

(Abstract of *J. Applied Phys.*, in press)

An "atom buncher" for controlling the concentration of gaseous samples has been conceptualized, evaluated theoretically, fabricated, and tested with excellent results. In effect, the atom buncher greatly increases the probability that a free atom will be in a small detector volume at a desired time. This was accomplished by using cryogenic techniques to condensate atoms on a small spot and a pulsed laser to momentarily heat the spot to release the atoms at the desired time. Our work on noble gas atom counting by using Resonance Ionization Spectroscopy (RIS) is discussed as one example of the applications of the atom buncher.

[*] Research sponsored by U.S. DOE Office of Health and Environmental Research and the Swiss Nationale Genossenschaft fur die Lagerung radioaktiver Abfalle (NAGRA).

[†] Chemical Physics Section, Health and Safety Research Division.

[‡] University of Bern, Bern, Switzerland.

1.63

AFTERPULSES AT SEVERAL μsec FOR AN RCA-8854 MULTIPLIER[*]

C. H. Johnson[†] N. W. Hill[‡]
J. A. Harvey D. J. Horen[†]

[Abstract of *Bull. Am. Phys. Soc.* 28(7), 992 (1983)]

At the ORELA time-of-flight facility we have extended the energy for neutron detection down to 5 keV for liquid or plastic scintillators by accepting pulses corresponding to a few photoelectrons. At such low levels there is a background of afterpulses which occur in the photomultiplier, a 5-inch RCA-8854 PMT, several microseconds after the earlier detection of a neutron or γ-ray. To study these we placed a hydrogenous filter in the flight path to remove essentially all neutrons and leave only the narrow initial γ-ray burst and its afterpulses. The time spectrum of the afterpulses (after the 1.1 μsec clock dead time) shows sharp peaks at 1.15, 2.15, 2.4, 2.9, 5.65, and 6.3 μsec and much broader peaks at 4.5, 7.5, and 14 μsec. For the γ-ray burst, which includes γ-ray energies mainly below 1.5 MeV, there is a 14% probability that a detector event will have an afterpulse later than 1.1 μsec. The probability increases with initial pulse height. Presently we are investigating the use of two photomultipliers in coincidence for minimizing this background.

[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

[†] Physics Division.

[‡] Instrumentation and Controls Division.

1.64

A PARALLEL PLATE ^{10}B NEUTRON DETECTOR[*]

J. H. Todd[†] L. W. Weston
G. J. Dixon[‡]

(Abstract of *Nucl. Instrum. and Methods*, in press)

Parallel plate ionization chambers with vacuum deposited ^{10}B electrodes have been constructed and tested for ^{10}B plating thicknesses from 24 μg/cm^2 to 61 μg/cm^2. Pulse-height resolutions of the alpha particle and of the ^{7}Li fragment from the ^{10}B(n,α) reaction were measured using low-energy neutrons. The pulse-height resolutions of the chambers were found to be better than a theoretical analysis had indicated.

[*] Research sponsored by U.S. DOE Division of Reactor Research and Technology.

[†] Instrumentation and Controls Division.

[‡] 1981 Summer Participant, Oak Ridge Associated Universities, Oak Ridge, TN.

1.65

A DIGITAL PULSE-PAIR DETECTING CIRCUIT[*]

Z. W. Bell[†] J. W. McConnell[‡]
E. D. Carroll[§]

[Abstract of *Nucl. Instrum. Methods* 211, 551 (1983)]

A completely digital pulse-pair detecting circuit is described. The inspection interval ranges from approximately 100 ns to 1.3 ms in steps of 20 ns. Tests of the circuit indicate reliable operation at input rates up to 25 MHz.

[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

[†] UCC-ND Computer Sciences Division.

[‡] Physics Division.

[§] Instrumentation and Controls Division.

1.66

NEUTRON FLUX MEASUREMENTS AT THE 22-METER STATION OF THE OAK RIDGE LINEAR ACCELERATOR FLIGHT PATH NO. 8[*]

Z. W. Bell[†] J. K. Dickens
J. H. Todd[‡] D. C. Larson

(Abstract of ORNL/TM-8514, May 1983)

The measurements of the ORELA flux at neutron energies from 0.16 to 31 MeV are described. The techniques of fitting calculated responses to measured responses and the method of calculating the covariance matrix are detailed. The measured neutron flux is presented.

[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

[†] UCC-ND Computer Sciences Division.

[‡] Instrumentation and Controls Division.

1.67

CALCULATION OF THE ORELA NEUTRON MODERATOR SPECTRUM AND RESOLUTION FUNCTION[*]

C. Cocera[†] R. Simonini[†]
D. K. Olsen

[Abstract of *Nucl. Instrum. Methods* 211, 459 (1983)]

The yield, spectrum, and delay-time distributions (resolution function) of escape neutrons from the ORELA water-moderated and water-cooled tantalum target assembly are calculated using time-dependent three-dimensional Monte Carlo techniques. The resulting spectrum and delay-time distributions of the moderated neutrons are compared with measured values.

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[*] Research sponsored by U.S. DOE Division of Reactor Research and Technology.

[†] Dell'Energia Nucleare e Delle Energie Alternative, Bologna, Italy.

1.68

A PROPOSAL FOR REPLACING THE ORELA PDP-10 COMPUTING SYSTEM[*]

D. C. Larson J. G. Craven[†]

(Abstract of a proposal submitted to U.S. DOE Basic Energy Sciences Program, May 24, 1983)

This proposal documents the history of the present DEC PDP-10 located at the Oak Ridge Electron Linear Accelerator (ORELA) and outlines problems with the current system, now 14 years old. Three possible solutions to the problems are presented and examined in detail. Finally, a possible system to meet the ORELA computing needs for the next 15 years is presented, along with cost estimates and factors of improvement over the existing system.

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[*] Research sponsored by U.S. DOE Office of Basic Energy Sciences.

[†] UCC-ND Computer Sciences Division.

8.6 Shared Research Equipment Program (SHaRE)

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

   Answer: This facility has a unique collection of microstructural and microanalytical instruments that allows the defect, crystal, and chemical structure of materials to be analyzed at a resolution of a few atomic dimensions. Studies of the changes in these structural features that occur as the material is subjected to extreme temperatures and stresses provide a basis for the prediction of service lifetimes, for establishment of performance limits, and the scientific design of improved materials.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

   Answer: Individual items of equipment present in this facility are present in other laboratories, but it is the collection of state-of-the-art instruments in one facility that allows the complete characterization of a materials structure on an atom by atom basis.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

   Answer:

Instruments and Facilities	Characteristics	Notes Regarding Application
Hitachi HU-1000 High Voltage Electron Microscope	Heating stages; in-situ deformation stages; low light level videorecording system; environmental cell—0.1 atm; 0.3 to 1.0 MeV	In-situ irradiation, deformation and gas-metal reaction studies
Philips EM400T/FEG Analytical Electron Microscope	TEM resolution <0.16 nm: STEM resolution <1.0 nm; energy dispersive x-ray analysis; electron energy loss spectroscopy: convergent beam electron diffraction	Structural and elemental microanalysis; minimum probe diameter <1 nm
JEOL 120CX Analytical Electron Microscope	TEM resolution ~0.34 nm; STEM resolution ~3 nm; energy dispersive x-ray analysis; electron energy loss spectroscopy	Structural and elemental microanalysis; minimum probe diameter <10 nm
JEOL 120C Transmission Electron Microscope	TEM resolution ~0.34 nm: special polepiece for TEM of ferromagnetic materials	Structural microanalysis; unique features required for studies of magnetic materials

Instruments and Facilities	Characteristics	Notes Regarding Application
Philips EM430 Analytical Electron Microscope	High resolution TEM with electron energy loss spectroscopy and energy dispersive x-ray analysis	To be installed June 1984
Imaging Atom Probe	Atomic level resolution and one atom chemical analysis	State-of-the-art instrument to be installed September 1984
PHI 590 Scanning Auger Electron Spectroscopy System	200 nm beam size; fracture stage; residual gas analysis; sputter depth profiling: elemental mapping	Surface analytical and segregation studies
Varian Scanning Auger Electron Spectroscopy System	5 μm beam size; hot-cold fracture stage: residual gas analysis; sputter depth profiling; elemental mapping	Surface analytical and segregation studies; gas-solid interaction studies
Dual Ion-Beam Accelerator Facilities	4 MW Van de Graaff accelerator; 400 kV accelerator; sputter depth profiling	Nuclear microanalysis; Rutherford backscattering: elemental analysis

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer:

FY 1981-82 (with D. R. Clarke, Rockwell International Science Center, Thousand Oaks, CA): Electron energy loss spectroscopy (EELS) was applied to the study of ceramic material (Si_3N_4) for the first time. By the use of EELS, energy dispersive x-ray spectroscopy, and advanced microdiffraction techniques, one amorphous and three crystalline phases were identified and the composition of each determined. These results resulted in a more complete understanding of the role of sintering aids in the consolidation of this technologically important ceramic.

FY 1983 (with R. F. Davis and C. H. Carter, Jr., of North Carolina State University. Doctoral dissertation of Carter): Transmission electron microscopy observations were correlated with creep data for two grades of silicon carbide (SiC). The microscopy observations enabled a description of the creep process to be developed in terms of local atomic processes. This material has great potential for application in a number of energy systems.

FY 1984 (with R. B. Benson and L. D. Stephenson of North Carolina State University. Doctoral dissertation of Stephenson): The microstructure of aluminum ion implanted with molybdenum is being determined for correlation with corrosion studies of the same material. Such studies may explain the altered corrosion behavior effected by ion implanting surface layers and lead to improved alloys.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: FY 1981

Upgrade of data acquisition system ($25K).

FY 1982

(a) Funds appropriated and order placed for Philips EM430 Analytical Electron Microscope to be used for high resolution lattice imaging studies and microchemical analyses ($350K BES-Materials Sciences, $250K Fusion Energy, $50K Breeder Reactor).

(b) Special specimen holder for microanalytical studies ($20K).

FY 1983

(a) Upgrade of data acquisition systems ($25K).

(b) Advanced specimen preparation facilities ($50K).

FY 1984

(a) Installation of equipment authorized in FY 1982.

(b) Special specimen preparation equipment for ceramic samples ($65K).

(c) Imaging Atom Probe ($225K BES-Materials Sciences, $225K Fusion Energy, $50K Conservation).

FY 1985

(a) High resolution analytical electron microscope to replace aging equipment ($250K BES-Materials Sciences, $400K Other DOE sources).

(b) Development of two-element analysis capability for imaging atom probe ($75K).

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer:

B/A
(Dollars in Thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Facility maintenance and supplies (Materials Sciences)	50	50	60	60	70
ORNL staff acting as collaborators with users (Materials Sciences)	125	130	150	165	190
ORNL technician support for users (Materials Sciences)	45	50	50	55	60
Staff support provided by BES-Materials Sciences through ORAU	40	45	50	55	58
In-house research					
BES-Materials Sciences	900	1000	1292	1680	1930
Fusion Energy	190	200	200	220	250
Breeder Reactor	200	150	100	50	50
Fossil Energy	20	30	50	60	70
Conservation	0	0	75	80	85
Outside research					
Other Federal Agencies, (Air Force Weapons Laboratory)	0	62	0	0	0
Westinghouse-Bettis	0	60	25	0	0
Materials Science support of users through ORNL and ORAU (costs not covered above)	10	10	22	37	45
SHaRE industry and university users	These scientists obtain their own funding through NSF, DOD, DOE, etc. The actual funding involved cannot be easily determined. An estimate based on number of faculty and students is provided. Some of the work of course is conducted at the university sites.				
	800	900	1000	1100	1150
Capital equipment					
BES-Materials Sciences	25	370	75	290	325
Fusion Energy	0	250	325	0	0
Breeder Reactor	0	50	0	0	0
Conservation	0	0	0	50	150
ARIM	0	0	325	0	0

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer: No direct funds received or expected.

8. **For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.**

Answer:

(Person years)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
ORNL technical collaborators	1.5	1.5	1.5	1.5	1.5
ORNL technicians	0.5	0.5	0.5	1.0	1.0
ORAU technical staff	1.0	1.0	1.0	1.0	1.0
In-house research					
Materials Science	9.0	10.0	12.0	14.0	15.0
Fusion	2.0	2.0	2.0	2.0	2.0
Breeder Reactor	2.0	1.5	1.0	0.5	0.5
Fossil	0.3	0.5	0.5	0.5	0.5
Conservation	0	0	0	0.5	1.5
Total	16.3	17.0	18.5	21.0	23.0

9. **What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?**

Answer: Current use is four 8-hour day shifts plus some week-end and night shifts. One other 8-hour shift is used for routine maintenance. Additional use for more night shifts requires additional staffing for collaboration and maintenance. Eight 8-hour shifts are theoretically possible. Certain items of equipment (such as specimen preparation items) are now used around the clock seven days per week. Additional demands would require additional equipment.

10. **For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?**

Answer: Not applicable. The research conducted in this facility consists of gathering information from a large number of samples that have been previously subjected to some thermal or mechanical treatment or exposed to some aggressive environment. Such studies tend to cover relatively long periods of time as opposed to discrete experiments.

11. **What is this facility's user policy?**

Answer: Letter proposals briefly describing collaborative research are submitted to the SHaRE Executive Committee for consideration. Approval is based on scientific excellence, previous research record of the proposers, relevance to DOE needs, and budget considerations. Access by users not requesting support from the ORAU SHaRE Program has always been granted subject only to limitations imposed by availability of the in-house staff.

8.7 Surface Modification and Characterization Laboratory

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

   Answer: The SMAC facility utilizes ion beams and pulsed lasers for fundamental materials research and development. Ion implantation doping, ion induced materials interactions, and pulsed laser annealing are all nonequilibrium materials processing techniques. Consequently, they can lead to new and often unique materials properties not achievable by normal materials processing methods. These techniques have led to the development of new metastable alloys, supersaturated solutions, amorphous mixtures, metglass formation and unique lattice alterations. Intense defect production and interactions resulting from ion irradiation provide a new processing variable for inducing materials interactions, and pulsed laser annealing leads to ultra rapid solidification 10^2 times greater than splat quenching. Consequently, these techniques are ideal for fundamental materials research because they lead to new materials and force materials interactions to new limits. They are also ideal surface modification techniques for practical applications. They have been used to passivate metals against corrosion and oxidation, fabricate semiconductor devices and solar cells, reduce friction and wear of metal parts, improve the hardness and fracture toughness of ceramic surfaces and even improve corrosion-wear of surgical alloys. The scientific opportunities are in fundamental materials research, practical surface modification of materials, and in technology transfer.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

   Answer: The unique feature of the SMAC facility is the integration of a variety of ion accelerators and lasers into common ultrahigh vacuum chambers where materials processing and in situ materials analysis can be performed. Consequently, it is possible to alter the properties of virtually any material by ion implantation doping, ion beam mixing, and pulsed laser annealing in an ultrahigh vacuum environment at sample temperatures from 4-1500° K and to analyze the properties of the material in situ by ion beam, laser and surface analysis techniques. These unique capabilities are invaluable for fundamental materials studies and for proof-of-principle experiments in assessing surface modifications for practical applications.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

   Answer: The SMAC facilities include:

   1. 2.5 MV Van de Graaff accelerator.
   2. 1.7 MV Tandem-type accelerator.
   3. 40-400 keV high current ion implantation accelerator.
   4. 0.1-40 keV direct ion deposition system.
   5. Q-switched ruby laser (10^{-9} s).
   6. KrF pulsed laser (10^{-9} s).
   7. Ultrahigh vacuum processing and analysis chambers (10^{-7}-10^{-11} Torr).
   8. Variable temperature sample manipulators (4-1500 K).
   9. Ultrahigh vacuum goniometers.

   The capabilities include:

1. Ion implantation doping.
2. Ion beam mixing.
3. Pulsed laser annealing.
4. Direct ion beam deposition.
5. Simultaneous dual ion beam irradiations.
6. Combined alteration and analysis in situ in ultrahigh vacuum environments.
7. Ion beam analysis (ion scattering, channeling, ion induced nuclear reactions and characteristic x-rays).
8. Surface analysis (LEED, AES).

4. What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?

Answer: Research highlights achieved during the period FY 1981 through the middle of FY 1984 included the following:

1. U.S. Department of Energy award for outstanding sustained research (1981).
2. IR-100 Award for Supersaturated Substitutional Alloys.
3. Formation of Supersaturated Substitutional Alloys by Ion Implantation and Laser Annealing, seventh most cited reference in materials science for 1982.
4. Determination of the mechanisms limiting substitutional solubilities in silicon at ultra-rapid growth velocities.
5. Time resolved x-ray diffraction measurements of interface temperatures and thermal gradients during rapid solidification.
6. Metastable surface structures on (111) silicon produced by laser annealing.
7. Surface electronic properties of supersaturated alloys produced by ion implantation and laser annealing.
8. High efficiency solar cells produced by ion implantation and laser annealing.
9. Unique morphological instability induced in Ge during ion irradiation.
10. Studies of fundmental ion beam mixing mechanisms of metal films on silicon.
11. Reduction of electrochemical corrosion of Ti by ion implantation.
12. Reduction of wear on surgical alloys by ion implantation.
13. Effect of ion implantation on the near surface mechanical properties of ceramics.

Results expected for the remainder of 1984 and 1985 include:

1. Direct ion beam deposition of metal, semiconducting, and insulating films.

2. Ion beam mixing of metal films on silicon: effect of interface impurities.

3. Formation of buried insulating layers in silicon by high dose and high dose rate ion implantation.

4. Substitutional solubility limits achieved by laser annealing and laser induced diffusion.

5. Model to explain unique morphological instability in ion irradiated Ge.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: The equipment and building additions associated with the SMAC facility were:

FY 1981

1. Addition of laboratory and office space to east end of existing facility ($400,000, ORNL GPP funds).

2. Relocation of ion implantation accelerator and establishment of two additional UHV beam lines ($250,000 capital equipment funds).

FY 1982

1. Addition to west end of SMAC facility to provide laboratory space for new accelerator ($245,000 ORNL GPP funds).

2. New 1.7 MV tandem accelerator/implanter ordered ($656,000 capital equipment funds).

FY 1983

1. New building for SMAC Laboratory and Collaborative Research Center ($650,000 ORNL GPP funds).

FY 1984

1. New 1.7 MV tandem accelerator/implanter installed.

2. Two complete UHV beam lines and analysis stations ordered for SMAC facility ($500,000 capital equipment funds).

FY 1985

1. New two story addition will be added to SMAC facility to provide computer room and lab space for users ($500,000 ORNL GPP funds requested).

2. New high current ion implantation accelerator and beam line ($825,000 capital equipment funds requested).

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer:

	B/A In Thousands				
Item	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operations					
BES Material Sciences	$ 0	$ 0	$ 460	$ 500	$ 850
In-House Research	982	1,478	1,295	1,345	1,405
BES--Material Sciences	857	1,283	1,120	1,220	1,280
OFE-ER	125	195	125	125	125
DOD-Army	0	0	50	0	0
Out-of-House Research*	0	0	400	400	600
Other Operating Expense	70	0	0	200	0
Capital Equipment--BES	99	633	257	595	825
AIP	0	0	0	0	0
General Plant Project--OFE	0	235	235	650	500
In-House Energy Management	0	0	0	0	0
Other Construction	0	0	0	0	0
TOTAL	$1,151	$2,346	$2,647	$3,690	$4,180

* This research is funded by sources in NSF, DOD, Other DOE and Industry, etc. and obtained by the institutions doing the research and is usually not known by ORNL.

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer: The majority of all funding for the SMAC facility and the associated research programs comes from the Office of Basic Energy Sciences, Division of Materials Sciences, USDOE. Through FY 1983 only $50,000 was supplied by other federal agencies (U.S. Army) and $50,000 from private sources (industry). No significant change is anticipated through FY 1985. All indirect funding (e.g., travel, living expenses, sample preparation, etc.) for users is furnished by the users' institutions or by grants from federal agencies to the users.

8. **For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.**

Answer:

SMAC FACILITY STAFF
(Established as User Facility FY 1984)

FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
6.0	7.0	8.5	10.0	11.5

9. **What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?**

Answer: Because of the demand by SMAC facility staff and outside collaborators for experimental time on the ion accelerators and lasers, the facilities are scheduled 7 days per week including holidays. Full utilization (100%) is based on 40 hours per week. Using estimates from timers on the accelerators it is estimated that the facility utilization is 140%. This increasing demand for experimental time is the basis for the expansion of SMAC facilities.

10. For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?

Answer: The number of experiments involving SMAC facility personnel and outside collaborators from universities, industry, other government laboratories in the US and foreign institutions which were started, continued, and completed for the period FY 1981-1984 is estimated to be 600.

11. What is this facility's user policy?

Answer: Because of the complex nature of the materials alteration and analysis capabilities of the SMAC facility it is difficult for uninitiated users to benefit from independent utilization of the facility. Consequently, the SMAC Collaborative Research Center operates primarily in a collaborative mode where outside researchers work with SMAC facility staff. This policy insures efficient and safe utilization of the facilities; enables outside users to benefit from the cumulative expertise of SMAC staff in solving their particular problem quickly; and results in rapid and realistic technology transfer by doing proof-of-principle experiments on each user's particular materials problem. In the past, outside users have been accommodated through informal contacts with members of the SMAC staff. However, a more formal policy, involving written proposals and a proposal review committee, has been established recently (see Question 13).

The SMAC CRC also has provisions for doing proprietary research on a full-cost-recovery basis.

12. For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?

Answer: The SMAC facility began operation as a true users' facility only in FY 1984, although extensive collaborative research occurred prior to that on an informal basis.

13. What is the mechanism by which specific research proposals for experiments at the facility are considered?

Answer: Proposals are submitted to the director of the SMAC Collaborative Research Center. An internal ORNL review committee insures that the proposed work can be done at SMAC, that the work is within the scope of DOE, and that the work is not in conflict with the private sector. A qualified researcher is identified from the SMAC CRC staff for each proposal accepted. All proposals are then submitted to a program committee composed of distinguished scientists from outside institutions who have a broad perspective on materials science and are familiar with the capabilities of SMAC. This program committee evaluates the scientific merit and prioritizes the proposals.

Once a proposal is accepted, the CRC staff member on the proposal schedules experimental time on SMAC and serves as liaison and collaborative research partner for the outside user.

14. How many research proposals have been submitted over the past five years, and how many of these have been approved?

Answer: As stated earlier the SMAC Collaborative Research Center is being formalized in FY 1984 as a collaborative research center so there have been no formal submissions of research proposals. If the informal collaborative research over the past five years is analyzed there have been approximately 80 collaborative projects with research scientists from universities, industry, other national laboratories, and foreign institutions.

15. How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?

Answer: In the past five years approximately 25 university personnel have utilized the SMAC facilities. Many of them have used the facilities several times during this period.

16. How many industrial researchers have utilized the facility over the past five years?

Answer: In the past five years approximately 20 industrial researchers have utilized the SMAC facilities. Many of them have used the facilities several times during this period.

17. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer: In the past five years approximately 25 researchers from foreign institutions have utilized the SMAC facilities. Several of them have used the facilities for more than one experiment.

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: In the past five years approximately 8 researchers from other agencies in the US have utilized the SMAC facilities. Some of them have used the facilities several times during this period.

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: There are many potential future development possibilities for the existing Surface Modification and Characterization Facility, but there are currently no specific plans to undertake any of them beyond the construction activities identified in the FY 1985 budget request.

20. Please provide a copy of the facility's latest annual report.

Answer: Since the SMAC CRC has only been functioning since FY 1984 it does not have an annual report. Because the work is collaborative and of a basic nature most of the results are published in the open literature.

8.8 Transuranium Processing Plant (TRU)

1. **What have been the facility's highlights for the period FY 1981 (or from start of operation if later than FY 1981) - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer: Transplutonium elements are recovered in the Transuranium Processing Plant (TRU) from curium oxide targets irradiated in the High Flux Isotope Reactor (HFIR). This is part of the DOE-ER heavy-element research program. TRU and HFIR provide the western world's supply of elements beyond curium (atomic number 96), either directly or by furnishing starting materials for further nuclear-synthesis reactions. Isotopes of berkelium, californium, einsteinium, and fermium are purified and distributed, primarily to researchers at the DOE National Laboratories, but, also, to approximately 30 other laboratories in the United States and a dozen around the world. A recent workshop at the National Research Council on "The Opportunities and Challenges in Research with Transplutonium Elements," has shown that there are at least five areas where important and challenging scientific problems can be solved only if products from HFIR and TRU remain available. Since many of these products are short-lived and cannot be stockpiled, we anticipate continuing the Transplutonium Element Production Program at about the same rate, through and beyond FY-85. Approximately 100 mg of Cf-252 is being furnished each year to the Savannah River Laboratory for use in Defense Programs activities. Some special shipments in recent years have been: samples of six isotopes for the Joint United States/United Kingdom Higher Actinides Irradiation Program; samples of Cm-243 for biological effects studies at the Lovelace Foundation; gram quantities of high isotopic purity Pu-240 for FFTF flux monitors and other neutron physics studies; special samples of Cf-252 for the preparation and study of short-lived nuclides from spontaneous fission fragments; large neutron sources (totalling 50 mg of Cf-252) for the Bettis Atomic Power Laboratory's LWBR Proof-of-Breeding Program; special Cf-252 fission chambers for new developments in criticality studies; and a sample of Ac-227 to serve as a generator of Ra-223 used in the 1983 Nuclear Weapons Accident Exercises by the Defense Nuclear Agency. We anticipate continuing these special activities in FY-84 and FY-85, although the exact products will depend on the needs of researchers.

A Solvent Extraction Test Facility (SETF) is operated in one of the TRU hot cells to (1) develop and demonstrate the suitability of conceptual flowsheets for the solvent extraction processing of LWR and breeder reactor fuels and (2) evaluate process control instruments and procedures. This program, which is part of the DOE-NE Consolidated Fuel Reprocessing Program, constitutes approximately 17% of the total effort at TRU. Since FY-81, emphasis has been on breeder fuel reprocessing using fuels irradiated in the EBR-2, the General Electric Test Reactor, and the Fast Flux Test Facility (FFTF). This activity is expected to continue through and beyond FY-85 using high burnup FFTF fuel to evaluate solvent extraction flowsheets and provide recycle plutonium for fuel fabrication and reirradiation studies.

We have been involved since 1979 in the development of processes and techniques for various aspects of the recovery program for the Three Mile Island Unit 2 reactor. The capabilities of the TRU facilities and staff to handle highly radioactive materials have provided quick resolution of several important problems. This involvement is expected to continue through and beyond FY-85.

2. **What facility changes and additions have occurred or are anticipated for the period FY 1981 (or from start of operation if later) - FY 1985?**

Answer: No significant changes have been made and none are planned during the period FY-81 through FY-85.

3. **For the period FY 1981 (or from start of operation) - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer:

(Budget Authority In Thousands)

	FY-81	FY-82	FY-83	FY-84	FY-85
Total operating	3815	4292	4934	5221	5582
In-house R&D (NE)	1095	1175	1148	1157	1167
Total Operations	4910	5467	6082	6378	6749
Capital Equipment	43	87	91	95	50
TOTAL	4953	5554	6173	6473	6799
Support Operations:					
Nuclear Sciences (BES)	3740	4200	4800	5136	5490
Nuclear Energy	1095	1175	1148	1157	1167
Other	75	92	134	85	92
Total	4910	5467	6082	6378	6749
Capital Equipment:					
Nuclear Sciences (BES)	43	52	91	95	50
Nuclear Energy	0	35	0	0	0
Total	43	87	91	95	50

4. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer: Funding by other federal agencies and private sources has always been very small and arises in the form of payments for special services required for preparing, packaging, and handling certain research samples. For the period FY 1981 - FY 1985 these payments have averaged about $95,000 per year.

5. **For the period FY 1981 (or from start of operation) - FY 1985, please provide actual and estimated staffing levels.**

Answer:

	FY-81	FY-82	FY-83	FY-84	FY-85
Total FTE's	56	56	59	58	57

6. **What is the actual and estimated facility utilization for the period FY 1981 or from start of operation) - FY 1985? What would be defined as "full" utilization of the facility?**

   Answer: Facility utilization is not readily quantified, but since FY-81 there has been unused operations capability. We expect this to continue through FY-85. In terms of the production of heavy element research materials, TRU could about double its output under "full utilization". We consider "full utilization" to mean three or four major HFIR target processing campaigns per year, depending on maintenance requirements. Due to staffing and budget constraints beginning before FY-81, the processing rate in recent years has comprised three HFIR target campaigns each two years plus a series of DOE-NE fuel reprocessing solvent extraction flowsheet development tests each year. This is equivalent to a total of approximately two major processing campaigns per year.

7. **What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?**

   Answer: We have no present plans to develop the facility (except in certain areas relating to safety and environmental impact of operations). However, TRU is a flexible hot-cell facility for handling high levels of alpha, beta, gamma, and neutron radioactivity and has extensive glove-box facilities for performing research and development involving high levels of alpha activity. Hot cell equipment can be modified or replaced easily to permit substantial changes in programs or program emphasis. TRU has substantial potential to undertake programs to produce special heavy element isotopes or unusually large amounts of certain isotopes, and to initiate new programs as exemplified by the Solvent Extraction Test Facility.

8. **Please provide a copy of the facility's latest annual report.**

   Answer: A formal annual report is not available. The attached is the appropriate part of the ORNL Chemical Technology Division Progress Report for the period April 1, 1981 through March 31, 1983.

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Contract No. W-7405-eng-26

Chemical Technology Division Progress Report for the Period April 1, 1981, to March 31, 1983

R. G. Wymer, Division Director
C. D. Scott, Associate Division Director

Section Heads

J. R. Hightower	Advanced Technology
R. E. Leuze	Pilot Plant
A. P. Malinauskas	Chemical Development
W. W. Pitt, Jr.	Experimental Engineering
V. C. A. Vaughen	Engineering Coordination and Analysis
S. K. Whatley	Technical Support

Date of Issue—September 1983

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830
operated by
Union Carbide Corporation
for the
DEPARTMENT OF ENERGY

7. TRANSURANIUM-ELEMENT PROCESSING

The Transuranium Processing Plant (TRU) is the production, storage, and distribution center for the heavy-element research program in the United States. The transuranium-element isotopes produced at TRU continue to be used nationally and internationally in basic studies of the physics and chemistry of the transuranium elements, including experiments to produce new, super-heavy elements. Target rods irradiated in the High Flux Isotope Reactor (HFIR) are processed at TRU for the separation, recovery, and purification of the heavy actinide elements, which are distributed to laboratories throughout the country for their research work with these elements. Products are usually highly purified prior to shipment and are frequently provided in special chemical forms and/or in special devices required by the experimenter. In addition, TRU is the sole source of the ^{252}Cf that is distributed worldwide by the DOE californium program at the Savannah River Laboratory (SRL) and is used to prepare neutron sources for a variety of applications in industry and medicine.

7.1 TRU Operations

The purposes of this section are to report the production and distribution of transuranium materials and to describe recent changes in the processes and equipment being used in TRU.

Production and Shipment

During this report period, 40 HFIR targets were processed to recover the transuranium elements. Table 7.1 presents data on the amounts of key isotopes obtained during this 2-year period, as well as the total amounts produced at TRU in 15 years of previous operation. In addition to the HFIR target campaigns, ~1.8 g of curium, with a relatively high concentration (~8%) of ^{243}Cm, was purified and made ready for distribution. This curium had been recovered and partially purified, during the last report period, from six ^{241}Am slugs that had been irradiated at the Savannah River Plant (SRP).

Table 7.1. Amounts of materials recovered in the Transuranium Processing Plant

	April 1979 to March 1981	August 1966 to March 1979
Number of years	2	15
Number of target campaigns	3	41
Number of targets processed	40	474[a]
Amounts of key isotopes recovered		
^{242}Pu	0	141 g
^{243}Am	15 g	271 g
^{244}Cm	143 (293)[b] g	1980 g
^{249}Bk	104 mg	556 mg
^{252}Cf	1061 mg	4976 mg
^{253}Es	4.0 mg	23 mg
^{257}Fm	2.3 pg[c]	12 pg[c]

[a] The number of targets includes 277 HFIR targets, 176 SRP slugs and targets, and 21 SRP Pu-Al tubes.

[b] The value in parentheses is the total mass of all curium isotopes.

[c] Estimated amount.

Two batches of high-purity ^{248}Cm, containing a total of 340 mg of ^{248}Cm, were separated from the parent ^{252}Cf; another batch, containing 72 mg of ^{248}Cm that had been recovered previously, was further purified and made ready for distribution.

A total of 73 shipments of transuranium elements was made during the report period. The total amounts of each type of product shipped are listed in Table 7.2.

Processes and Equipment

A new processing step was added to the HFIR target campaign in order to recover a small amount of ^{95}Zr for later use as a tracer in several Solvent Extraction Test Facility (SETF) experiments. During a normal target campaign, the ^{95}Zr is quantitatively retained in the waste solvent [di-(2-ethylhexyl) phosphoric acid in Amsco diluent] from the Cleanex batch solvent extraction step.

Table 7.2. Amounts of transuranium elements shipped during the period April 1, 1981, to March 31, 1983

Major isotope	Total amount	Number of shipments
^{227}Ac	0.08g	1
^{244}Pu	3.2 mg	1
^{241}Am	*a*	1
^{243}Am	106 mg	1
^{243}Cm (8%)	12 mg	2
^{243}Cm (58%)	0.8 mg	3
^{244}Cm (72%)	275 mg	1
^{246}Cm (66%)	54 mg	1
^{248}Cm (97%)	106 mg	7
^{249}Bk	66 mg	9
^{249}Cf	28 mg	8
^{252}Cf	297 mg	25
^{253}Es (mixed)	2.4 mg	5
^{253}Es (milked)	137 μg	4
^{254}Es	4.5 μg	2
^{257}Fm	1.9 pg[b]	2

[a] The neutron source AmBe-514, returned from Ames Laboratory as part of a group of sources destined for disposal (emits 2×10^6 neutrons per second), was shipped unaltered.

[b] Estimated.

The bulk of ^{95}Zr (~80%) was recovered by diluting the solvent with 2-ethylhexanol, heating to 50–60°C, and back-extracting the ^{95}Zr by several contacts with heated 0.5 *M* oxalic acid. The product solution was then treated to remove the oxalate by adding strong HNO_3 and heating for several hours. Only 10% of the ^{95}Zr remained in solution after this treatment, but this was enough for use in the tracer tests.

Target Fabrication

Thirty-six HFIR targets for transuranium-element production were fabricated from a mixture of curium and americium oxides. Feed material for these targets included recycled americium-curium mixtures recovered from irradiated HFIR targets, ~17 g of americium and ~1 g of curium that had been recovered from irradiated LWR fuel in the SETF, and ~106 g of curium that had been recovered at TRU during the Californium-I Program in 1972 and stored at the SRL. In addition, three special targets were fabricated: one containing ^{54}Fe and ^{118}Sn for the Operations Division, another containing stainless steel specimens for an irradiation test by the Metals and Ceramics Division, and a third containing ^{226}Ra for the special project discussed in the following section.

7.2 Special Projects

The facilities available at TRU are used for a variety of purposes in addition to those associated with the main-line production and distribution of transuranium elements. These special projects include nonroutine productions, special preparations, special irradiations in the HFIR, and fabrication of neutron sources from ^{252}Cf.

Fabrication of Neutron Sources from ^{252}Cf

Some of the californium recovered at TRU is incorporated into neutron sources that are loaned to researchers. Four sources, containing 0.4 μg to 56.6 mg of ^{252}Cf, were fabricated during this report period. One of these was doubly encapsulated in type 304L stainless steel in a standard TRU configuration (NSD),[1] which was then further enclosed in an aluminum can furnished by the customer. One source was singly encapsulated in type 304L stainless steel and will be used at TRU for calibration of the equipment used to assay californium. Another source was of a completely new design, although the pellet was fabricated using techniques similar to those for a National Bureau of Standards point source. The new design (designated model LSD) was certified as a special-form container and can hold more californium than existing models. This first LSD source contained 56.6 mg of ^{252}Cf, which is more than any other source previously made at TRU by a factor of ~2. Another special source, containing only 0.4 μg of ^{252}Cf, was made in collaboration with the ORNL Isotopes Research Materials Laboratory (IRML). This source, consisting of a $CfCl_3$ deposit encapsulated in a vanadium capsule (0.89 mm diam by 4 mm long) and attached to a wire, will be used to measure the reactivity of HFIR fuel assemblies.

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[1] J. E. Van Cleve, Jr., L. C. Williams, J. B. Knauer, and J. E. Bigelow, "Fabrication of Cf-252 Neutron Sources at Oak Ridge National Laboratory," p. 25 in *Applications of Californium-252*, Proc. of Am. Nucl. Soc. Topical Meeting, CONF-720902, 1972.

Sources Returned

Neutron sources are returned to TRU when the projects for which they were requested are completed or when replacements are ordered to make up for decay of the ^{252}Cf. These sources are available for reassignment until the appropriate time for reprocessing to recover the ^{248}Cm daughter. During the current report period, 10 sources were returned and 7 were reassigned; 83 are now on loan, and 22 (containing from <1 μg to 10 mg of ^{252}Cf) are available for reassignment.

Electroplated ^{252}Cf Fission Sources

Some varieties of fission sources were prepared by electroplating small amounts of purified californium from dry isopropanol solutions onto platinum foils or disks. The total of seven electrodeposited sources made during this report period contained from 5 to 800 μg of ^{252}Cf.

Preparation of ^{240}Pu

An ~30-g sample of ^{240}Pu, which was initially recovered during TRU Campaigns 59 and 60, was prepared for final distribution. This plutonium was first purified by a standard anion-exchange step and then converted to the oxide form by precipitation of plutonium oxalate, followed by calcination of the precipitate. Table 7.3 lists the isotopic composition of this product. Another batch of ^{240}Pu (containing 16 g) was removed from Campaign 63 and will be prepared for shipment later. The source for all of this ^{240}Pu was the curium from SRL that had been recovered at TRU in the early 1970s for the Californium-I program and then stored at SRL. During the past few years, this curium was returned to TRU, separated from the ingrown plutonium, and used to augment the feed for HFIR targets. Since the original composition was ~80% ^{244}Cm (18-year half-life) and ~18% ^{246}Cm (4600-year half-life), with essentially no ^{242}Cm, the plutonium that has grown into it over the past ~10 years is very high-purity ^{240}Pu, with only a small amount of ^{242}Pu; it is of interest to several customers.

Table 7.3. Isotopic composition of plutonium from Campaigns 59 and 60

Nuclide	Distribution (at. %)
^{238}Pu	0.0090
^{239}Pu	0.0030
^{240}Pu	99.872
^{241}Pu	0.0019
^{242}Pu	0.114
^{244}Pu	0.0006

Preparation of ^{227}Ac

Approximately 0.08 g of ^{227}Ac was produced by irradiation of 6 g of ^{226}Ra in the HFIR. The ^{227}Ac was transferred to the ORNL Operations Division, where ingrown ^{223}Ra will be recovered from the ^{227}Ac for the Defense Nuclear Agency. Prior to the irradiation, ~6.5 g of ^{226}Ra was recovered from a variety of discarded radium capsules and needles obtained from the Los Alamos National Laboratory, from the Eastern Environmental Research Facility of the EPA, and from a $RaBr_2$ capsule furnished by the Mound Laboratory. This radium was used to make a standard HFIR target that was irradiated for one cycle at full power. The target was then returned to TRU where it was cut into sections and dissolved. The actinium was purified from the radium by one batch solvent extraction run and several cycles of cation exchange and was subsequently transferred to the Operations Division.

Production Cross Section Measurements for ^{254g}Es

A special request was made for a 40-μg sample of ^{254g}Es.[2] Production of this amount of material in the HFIR by normal irradiation of standard HFIR targets is impractical because of the very low yields of this highly fissionable nuclide. As a prerequisite for designing a suitable production method, new cross section measurements on ^{253}Es and ^{254}Es in the thermal and epithermal energy regions must be obtained, since the existing published values are grossly inconsistent with the observed concentrations of ^{254g}Es in HFIR-irradiated targets.

An experimental program to measure the needed cross sections was developed in collaboration with the ORNL Chemistry Division. The first irradiation used a portion of the ^{253}Es milked from the Campaign 62 californium. The californium had previously been treated to remove ^{254g}Es that might obscure the production cross section measurements. Although only a minute quantity of ^{254g}Es remained after these separations, the ^{253}Es sample (20-d half-life) decayed to only ~20 ng by the time the material was placed in the reactor. Thus the long-lived ^{254g}Es became a significant contaminant in the sample, and an accurate production cross section for ^{254g}Es was difficult to determine. In spite of this problem, the experiment was continued in order to gain working experience. The einsteinium was carefully purified in microscale columns, and three ~5-ng portions were deposited on aluminum microplanchets. These were fabricated into a specially designed rabbit that included cadmium covers for two of the planchets, and the rabbit was then irradiated in the HFIR for 24 h. The reactor was operated at reduced power (33 MW) specifically for this irradiation period. The rabbit was then transferred to TRU and disassembled; the microplanchets were analyzed by the Chemistry Division. As anticipated, the original ^{254g}Es content of the sample prevented the collection of all of the desired data, although information was obtained on the cross sections for production of the short-lived ^{254m}Es and of the secondary capture product, ^{255}Es.

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[2] *Chem. Technol. Div. Annu. Prog. Rep. Apr. 1, 1979, to Mar. 31, 1981*, ORNL-5757, November 1981, p. 120.

A second experiment used the Oak Ridge Research Reactor to irradiate a fresh sample of ^{253}Es milked from Campaign 63 californium product. Results are not yet available for this second sample, but the ^{254g}Es content may again have been great enough to reduce the accuracy of the measurement, since a 2-month delay in the operation of the reactor resulted in a loss of ~90% of the ^{253}Es. A third sample has now been milked, also from Campaign 63 californium, using extraordinary efforts to minimize ^{254g}Es contamination. Irradiation of this highly purified sample is expected to result in a definitive measurement of the capture cross section to produce ^{254g}Es.

9.0 Sandia National Laboratories, Livermore Combustion Research Facility (CRF)

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

Answer: The CRF is the only facility in the world specifically designed and equipped to advance our understanding of important chemical reactions fundamental to combustion. Our unique lasers and novel laser techniques, coupled with our chemistry and mathematics research, are allowing us to make significant new contributions to: (1) determining the identity and role of chemical precursors on the formation of particulates, (2) elucidating the chemical mechanisms -- to a depth of understanding which includes important free radical intermediates OH (hydroxyl), CN (cyano), CH (methylidene), -- of pollutant formation in combustion, (3) discovering important new correlations between chemistry and fluid mechanics in turbulent reacting flow, and (4) revealing the effects of gas-phase chemistry on material properties.

Because this program is being carried out at a DOE Multiprogram Laboratory, we can focus a broad spectrum of research capabilities on a selected technology, emphasizing fundamental, long-range, high risk research with high potential payoff. As a result, we are carrying out basic research, with a quality second to none, in specific disciplines -- laser spectroscopy, chemical kinetics, quantum chemistry, computational mathematics are examples-- which are critical to furthering our knowledge in combustion.

The quality and breadth of resources -- especially the staff -- at the CRF are allowing us to attack some of the most difficult problems related to the kinetics and dynamics of combustion-related chemistry. For example, by combining the capabilities of the advanced laser systems at the CRF with recent developments in multi-dimensional array technology, we have been able to capture -- for the first time -- details of transient chemistry in propagating flames. The coupling of our experimental and theoretical chemistry programs, along with the development of numerical algorithms for computer modeling, have permitted us to make significant progress in unravelling some of the mechanisms which result in particulate and pollutant formation. We now are extending our research, by involving our surface science and materials programs, to gain an understanding of the effects of combustion phenomena on the corrosion behavior of materials in combustion environments. In the near future, we anticipate broadening of our program to study (1) fundamental issues leading to deposition on combustor surfaces, and (2) the basic mechanisms which control sulfur conversion on calcium carbonate in high-temperature environments.

The intimacy of our basic research with the conservation and fossil programs has provided BES with several important advantages. First, the direct conduit to industry provided by these programs provides us with early insights into critical industry problems. Second, these interactions offer the rare opportunity for efficient -- and meaningful -- technology transfer between basic research and industry. This relationship with industry is unique within the DOE and is regarded by some observers as exemplary.

Working with CRF tools in support of Conservation and Fossil-sponsored combustion research, we have made major advances (1) in understanding hydrocarbon emissions from internal combustion engines and (2) in exposing, for the first time ever, the details of devolatilization and combustion of coal particles and their relationship to temperature, oxygen concentration, additive concentrations and coal properties.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

Answer: First and foremost, the Combustion Research Facility (CRF) is the only facility in the US dedicated to fundamental research on combustion. Several similar efforts, patterned after the CRF, are appearing in Europe and Japan.

The CRF has established unique ways of technology transfer to industry. By setting up and fostering "working groups" on specific combustion topics (e.g., direct injected stratified charge, dilute homogeneous burn, knock, diesel combustion, slagging and fouling, ...) we get industry to bring their problems to meetings involving researchers from academia, national laboratories, and other industries. These working groups have been extremely successful in promoting meaningful transfer of knowledge and methods from the CRF to industry.

The CRF has resources for combustion science that do not exist anywhere else. Because of the central role lasers play in probing combustion-related phenomena, the CRF has designed and installed a unique computer-controlled periscope system that relays the output from each of the Facility lasers to any of fourteen research laboratories.

- The first Facility laser, DIANA, the most powerful pulsed dye laser in existence, was developed in a collaboration between Sandia and industry, resulting in an advancement of a factor of about ten in the state of the art in flashlamp-pumped dye laser technology.
- The second Facility laser, SIRIUS, is a unique suite of lasers optimized for the new generation of non-linear spectroscopies. We have recently demonstrated the unique ability to send centralized laser beams more than sixty meters to a research laboratory, where the beams are recombined with a spatial stability of a fraction of a micrometer. The resulting data were equivalent in quality to the best research experiments.
- Other unique Facility lasers are in the planning stage, including a next-generation tunable pulsed laser for multi-dimensional imaging studies, and an advanced-design excimer laser for photochemistry research.
- Individual experiments at the CRF are not duplicated elsewhere. The Vertical Turbulent Diffusion Flame is a large, vertical wind tunnel for studying the coupling between chemistry and fluid turbulence: this two-story high experiment, complemented with a number of laser probes, is unique in the world. Our high-pressure flame, optimized for the study of soot formation at pressures

characteristic of practical combustion, is the only one of its kind in the US. A unique multi-fuel, high-pressure combustor is under construction. In our studies of internal combustion in automotive engines, we have developed a single-cylinder research engine which has become a de-facto standard throughout the world. Many of our fundamental research experiments, especially those in laser spectroscopy, are of a complexity and sophistication not found elsewhere.

3. What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?

Answer: Research instrumentation/experimental devices available:

Technical Data on CRF

Equipment	Key Features
Flashlamp-pumped, tunable dye laser	Long pulse, high energy, high average power: 2 microsecond pulse length 5 Joules per pulse, 10 Hz Tunable 440 to 620 nm 0.03 nm bandwidth
Multi-purpose pulsed laser system	High peak power, high resolution doubled YAG and tunable dye lasers: Single mode capability, 10-500 mJ per pulse, 10-20 nanosecond pulse
Low pressure flames	10 microns to 1 atm. Mass spectrometer sampling probe
Atmospheric flames	Diffusion and premixed flames
High pressure flame	Combination of diffusion flame burner with high pressure flow chamber: Pressures up to 20 atm., slot-geometry burner, 2-0 laminar diffusion
Vertical turbulent diffusion flame	Open-circuit, induced draft wind tunnel with co-flowing axisymmetric fuel jet: 30 x 180 cm viewing section to 6000 scfm flow
Atmospheric Combustion Exhaust Simulator (ACES)	Atmospheric pressure combustion exhaust chamber: to 1200 degrees C, 0.5 - 100 m/s flow speed, trace species and particulates, optical and physical probes, materials test section

Equipment	Key Features
Combustion bomb	Simulates constant-volume engine combustion
Internal combustion research engines	Highly repeatable environment for homogeneous charge and diesel combustion studies
Experimental diagnostics research facilities	Laser fluorescence laboratory
	Coherent Raman spectroscopy laboratories
	Laboratory for laser ionization, saturation, optogalvanic detection of trace species
	Kinetics laboratories with tunable quasi-cw uv and ring dye lasers for analysis; excimer lasers for photolysis
Computing facilities	Minicomputers in laboratories Access to CRF VAX 11/780 Limited access to SNLL CRAY

4. What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?

Answer: Selected highlights of research accomplishments at the CRF since opening in March of 1981 include:

- CRF staff collaborated with Exxon scientists to devise an accurate chemical mechanism for the thermal $DeNO_x$ process - a process to remove NO_x pollutants. CRF contributions included the prediction -- subsequently verified by other groups -- of new reaction paths which were critical to the mechanism.

- CRF scientists have devised new experimental methods for determining the rates of elementary chemical reactions. In two independent but related efforts, improvements of an order of magnitude have been achieved, with the overall result of an increase in sensitivity of more than one hundred over "conventional" methods.

- An experiment designed by visiting scientists yielded the first practical two dimensional species-sensitive Raman images of turbulent flames.

- A researcher at the CRF independently discovered and demonstrated the polarization properties of coherent Raman spectroscopies. His results have constituted the basis for many of the improvements in CARS (Coherent Anti-Stokes Raman Spectroscopy) being demonstrated in laboratories around the world.

- Experiments at high laser powers revealed a new, previously undiscovered form of the interaction between molecules and high intensity electrical fields. This new form of Stark Effect was then used as a basis for a novel form of space-resolved infra-red spectroscopy.

- Experiments at the CRF's vertical turbulent diffusion flame have provided the first direct comparison of data and theory for the characterization of conserved scalars in non-premixed reacting turbulent media. In addition, the first direct measurements of scalar dissipation in turbulent reacting media were obtained and compared with theoretical calculations carried out by a visiting scientist at the CRF.

- The first quantitative two-dimensional maps of flames using laser-induced fluorescence were achieved in a steady, laminar flame. The method was extended to study the time-dependent evolution of an expanding flame front. We anticipate this kind of technology -- quantitative, two-dimensional characterization of the properties of a wide number of reacting systems -- to be a major emphasis of the CRF experimental research in the next few years.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: During the period FY 1981 - 1985 we have completely saturated the laboratory space within the CRF and have occupied another 14 laboratories inside the Sandia security area. Major experiments completed within the CRF include a multi-story turbulent diffusion flame, a chemical dynamics laboratory, a high pressure diffusion flame, and a new multipurpose central laser system, SIRIUS. A pressurized multi-fuels combustor is now under construction in the high-bay area. To accommodate our user demand we have converted the original general-purpose chemistry laboratory to a coal science laboratory. Our assembly room has been remade into a research laboratory for a university graduate student. This year we have added temporary trailers to house staff, previously located in the CRF, to free up space for an optics laboratory. To accommodate a one year visiting scientist from industry, we established a new laboratory for pulse combustion; due to shortage of space, this laboratory had to be built inside the security area.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer: Funding for the period FY 1981-FY 1985 for Facility: BES/Chemical Sciences:

(Budget Authority In Thousands)

Activity	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operations	1,900	1,930	2,170	2,490	2,750
In House Research	1,400	1,840	2,160	2,290	2,500
Out of House Research (Visiting Sci. Support)	300	480	680	730	770
Other Operating Exp	0	0	0	0	0
Capital Equip Funds	800	975	900	800	700
GPP Funds	0	0	0	100	530

Other Funding for In-House Research Conducted at the CRF

(Budget Authority In Thousands)

Source of Funds	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Other BES Support*	870	1,020	1,340	1,450	1,560
Conservation (DOE)	1,200	1,350	1,450	1,650	1,900
Fossil (DOE)	1,030	1,650	1,320	1,400	1,700
Defense Programs			500	750	1,000

* Funding shown is principally from "Materials" and "Engineering, Math and Geosciences."

7. How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?

Answer:

(Budget Authority In Thousands)

Source of Funds	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Nuclear Regulatory Commission	0	0	330	500	670
Industry Funds*	0	0	40	20	200

* Industry funding is from the Motor Vehicles Manufacturers Association (MVMA) and the Electric Power Research Institute (EPRI). The $200,000 in FY 1985 is the total anticipated from EPRI and MVMA.

8. For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.

Answer: Staffing Levels For BES/Chemical Sciences Combustion Research Facility Program

FTE's

Activity	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operations	19	16	16	17	18
In House Research	14	15	14	14	14
Out of House Research (Visiting Sci. Support)	2	4	5	5	5

These staffing levels do not include staff supported by funds identified in Question 6 above, and thus represent approximately one-half of the total Combustion Research Program at SNLL.

9. **What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?**

Answer: Facility Utilization

The Combustion Research Facility, originally designed for 14 user experiments, now contains 17 laboratories and 4 facility laser rooms. The percentage utilization of the laboratories has increased each year in the following fashion:

1981-1982...........47%
1982-1983...........71%
1983-1984..........100%
1984-1985..........120%

"Full utilization" for the CRF means a running experiment in each of the 14 original research laboratories. As indicated above, general purpose support facilities have been converted to experiments for users and visiting scientists.

Please note that in addition to the setups at the CRF, there are approximately 14 other combustion-related experiments located external to the CRF and, for the most part, inside the secure area at SNLL. These include some of our most complex, sophisticated experiments in diagnostics research, as well as our entire combustion materials effort, the atmospheric combustor (ACES), radiotracer chemistry, Fourier Transform Infra Red Spectroscopy, and others.

10. **For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?**

Answer: Because of the nature of the long-range basic research performed at the CRF by the in-house staff, it is difficult to adequately define the "start" and "stop" to experiments.

The CRF, initially sized for 14 research laboratories, now houses 17 experiments, at the cost of some of the general-purpose facilities (assembly area, chem. lab, etc.). Inside the secure area there are 14 additional combustion research experiments. Thus, since 1981, the Combustion Research Program has grown to accommodate some 31 experiments, 17 of which are located at the CRF. As is typical of new, individual research endeavors, these experiments are continuously being modified to accommodate changes suggested by the most recent results.

If we define an experiment as one in which a generalized goal has been accomplished and a final report issued, then 80 experiments have been started and completed while 30 experiments are continuing.

11. **What is this facility's user policy?**

Answer: Qualified scientists are encouraged to take advantage of the specialized resources available at CRF. Prospective participants should submit a brief proposal to the laboratory director. Criteria for selection include technical merit, the extent to which CRF facilities are utilized, overlap with DOE program objectives, and the availability of specific equipment. In general, the CRF will host visiting scientists to use the special-purpose lasers, work with resident staff, make use of computers and codes, and to set up experiments. Visitors receive no salary from Sandia and pay for their own travel, housing, meals, and other local expenses. Facility lasers, apparatus, technicians, instrumentation, computers, and the services of support groups are provided at no cost for research which is not proprietary. Research results from nonproprietary projects are expected to be published and disseminated. For scientists with active government contracts, support for CRF research often can be arranged on an informal basis with the contract manager. There are opportunities for faculty, post-doctoral scientists, and graduate students to obtain Sandia support for combustion-related research at the CRF. In specific instances, proprietary research can be carried out at the CRF. For this type of work, the DOE will be reimbursed on a full cost recovery basis for the use of all CRF resources. Details of a DOE Class Waiver for patent rights are available.

12. **For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?**

Answer: No reimbursable work has been done at the Combustion Research Facility, nor is any planned.

13. **What is the mechanism by which specific research proposals for experiments at the facility are considered?**

Answer: Prospective participants submit a brief proposal to the laboratory director. Criteria for selection include technical merit, the extent to which CRF facilities are utilized, overlap with DOE program objectives, and the availability of specific equipment. Proposals are reviewed in light of the identified criteria. The facility director is responsible for the acceptance or rejection of proposals.

14. **How many research proposals have been submitted over the past five years, and how many of these have been approved?**

Answer: The Combustion Research Facility has been in operation for 3 years. There have been approximately 65 proposals submitted by prospective visiting researchers. These requests were to establish residence at the CRF for a month or longer. Some 60 of these proposals have been approved.

15. How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?

Answer: In the three years of operation, the number of university personnel who have participated in technical activities at the CRF for a week or longer is 164.

16. How many industrial researchers have utilized the facility over the past five years?

Answer: In the three years of operation, the number of industrial researchers who have participated in technical activities at the CRF for one week or longer is 100.

17. How many researchers from foreign institutions have utilized the facility over the past five years?

Answer: Approximately 70 foreign visitors have utilized the facility for a period of one week or longer over the 3 year period of operation.

18. How many researchers from other agencies have utilized the facility over the past five years?

Answer: During the first three years of operation of the CRF there have been approximately 30 government users of the facility spending one week or longer. We estimate about one-third of these are from government agencies other than DOE.

19. What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?

Answer: There are many potential future development possibilities for the existing Sandia National Laboratories, Livermore Combustion Research Facility, but there are currently no specific plans to undertake any of them beyond the construction activities identified in the FY 1985 budget request.

20. Please provide a copy of the facility's latest annual report.

Answer: The annual report for 1982-1983 is attached. [Note: Excerpts from this report follow.]

SANDIA COMBUSTION RESEARCH PROGRAM

ANNUAL REPORT

1982—1983

An Account
of Fundamental and Applied Combustion Research
Carried Out During the Calendar Year

D. L. Hartley
Director of Combustion Sciences
Combustion Research Facility

Scientific Editor, M. A. Gusinow

Prepared by Sandia National Laboratories, Livermore, California 94550
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AN OVERVIEW OF SANDIA COMBUSTION RESEARCH

D. L. Hartley, Director

This collection of research highlights represents output of the Combustion Research Facility staff during their first two full year's occupancy in the new center. Since 1974 we have been developing as broad set of combustion research activities, which are now nearing a mature state of scientific productivity. The work of our in-house research staff and visiting scientists, supported with the most modern experimental and computational capabilities in the world, now contributes to many areas of energy-related combustion science, industrial process, and commercial product design.

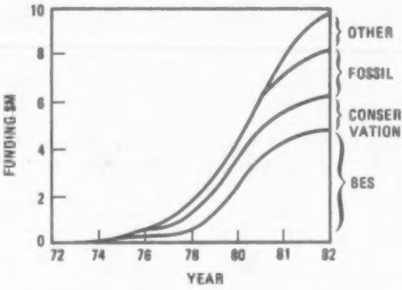
The construction of the Combustion Research Facility was sponsored by the Office of Basic Energy Sciences of the Department of Energy; and our charter is to promote the development and application of new combustion research tools, laser diagnostics in particular, with the active involvement of the combustion research community at large. In pursuit of this objective we have developed a fundamental research program in combustion sciences and laser diagnostics to complement our facility operation and to provide the experimental and analytical capabilities necessary for investigating critical and timely combustion problems. Visiting scientists from U.S., as well as foreign, research institutions are invited to join in these research efforts; and a healthy visitor program has evolved, resulting in continuing dialog with numerous combustion research centers around the world.

To further strengthen the relation of the program to current needs, and to make its special capabilities useful to the more applied missions of the Department of Energy, parallel research programs have also been developed under sponsorship of the Offices of Conservation and Fossil Energy. These efforts, which together roughly equal the scale of the BES program, emphasize the application of special research tools to internal combustion engines and to coal combustion problems, respectively.

The evolution of these programs, shown in the figure below, reached a funding level of about $10M per year by 1983.

Our broad involvement in fundamental and applied combustion science has created a research environment which we expect will continue to attract outside scientists to the Combustion Research Facility to participate in the work. This program, together with our unique facilities, a diverse and talented staff, and a vigorous continuing dialog with auto and combustor manufacturers as well as with university scientists, provides an opportunity to apply state-of-the-art research methods to critical problems in combustion, and to make the results available to designers in a timely fashion. Our primary intent is to couple our own capabilities with those of the combustion research community in a manner that will best ensure a meaningful contribution toward solving this nation's energy problems.

This annual report presents the results of these efforts for the calendar years 1982-1983. We trust they will be useful to the readership.



Combustion Funding at Sandia National Laboratories Livermore.

SECTION I FACILITIES AND SPECIAL EQUIPMENT

The Combustion Research Facility is a 51,500 square-foot, four-building complex forming an eastward extension of Sandia National Laboratories, Livermore. The Facility, which includes an office building, laboratory, auditorium, and mechanical equipment building, was designed to provide experimental and analytical equipment for the resident staff and visiting researchers. It is located outside the Sandia security area to permit easy access for visitors.

A number of unique features have been incorporated in the facility: two central facility laser systems which provide state-of-the art diagnostics capabilities, computers ranging from minis and superminis to main-frame systems, and a sophisticated microprocessor-controlled laboratory safety system.

An important role of the Combustion Research Facility in the combustion community is manifested in a vigorous program of interaction with other laboratories, primarily pursued through an extensive visiting scientist program and through cooperative research efforts with industry.

DEVELOPMENT OF THE SIRIUS FACILITY LASER: A CENTRAL LASER FOR REMOTE CARS

R. L. Farrow, R. P. Lucht, C. B. Layne

The Sirius laser system has been developed to provide state-of-the-art laser diagnostics to multiple users in the Combustion Research Facility. This laser will be used primarily for nonlinear techniques such as CARS (coherent anti-Stokes Raman spectroscopy) and IRS (inverse Raman spectroscopy) The remote application of CARS saves the considerable time and expense required to develop complete systems of this type in various CRF laboratories. The Sirius facility is presently equipped with a Molectron MY34 Nd:YAG laser, a Lamda Physik FL2002 dye laser, and a broad-band dye laser. The Nd:YAG laser is frequency-doubled and serves both as a pump laser for the dye lasers and as the pump beam for CARS experiments.

To perform CARS experiments in various CRF laboratories, the dye and YAG beams are sent from the Sirius facility to the user laboratory through the periscope system. A data acquisition system in the user lab communicates with a VAX 11/730 computer in the Sirius laser facility to control all necessary laser functions and to store data. Remote CARS has been demonstrated in a laboratory at the opposite end of the CRF, approximately 30 meters from the Sirius Facility. Figure 1 shows a CARS spectrum obtained from nitrogen in a flame in the remote laboratory. The signal-to-noise ratio of the spectrum is not noticeably affected by propagating the pump and dye beams the length of the building.

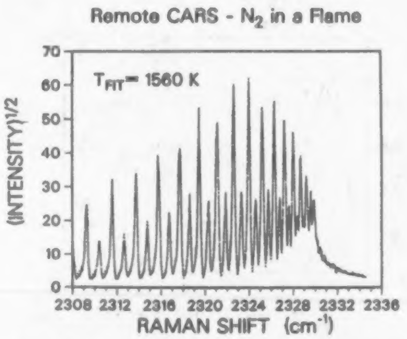


Fig. 1. CARS spectrum of nitrogen in a flame obtained by using periscope system to send beam pump and dye laser beams to a remote laboratory.

The Nd:YAG laser can be operated with either multiaxial or single-axial-mode frequency output. The single-mode Nd:YAG laser has a very narrow bandwidth (< 0.01 cm^{-1} at 1.06 μm) and a smooth temporal pulse shape with an FWHM of approximately 20 ns. With multimode operation the Nd:YAG laser has a linewidth approximately ten times greater, and beating between axial modes produces fast temporal modulation of the laser pulse. Because of the nonlinear power dependence of the CARS interaction, temporal modulation of the pump beam results in significant pulse-to-pulse fluctuations in CARS intensity.

Recent CARS experiments with the single-mode Nd:YAG laser show that pulse-to-pulse noise in single-shot CARS signals is considerably reduced relative to the multimode case. A comparison of single-shot statistics of CARS signals for single-mode and multi-mode Nd:YAG pump laser radiation is shown in Fig. 2. The rms standard deviation of the measurements is 7 percent in the single-mode case, as opposed to 100 percent in the multimode case. The disadvantage of operating the Nd:YAG laser with a single axial mode is that the pulse energy at 532 nm is almost a factor of three lower than in multiaxial mode operation. However, if necessary, Nd:YAG amplifier rods

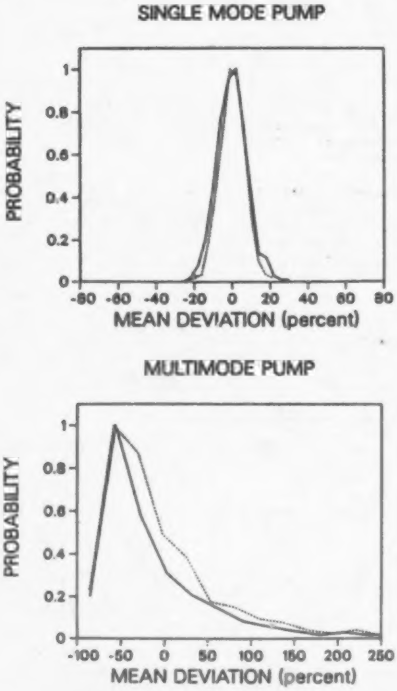


Fig. 2. Comparison of single-shot statistics for CARS intensities using (a) single-axial mode and (b) multiaxial mode Nd:YAG pump beam. The dashed curve represents measurements normalized by the probe and squared pump laser energies; the solid curve is not normalized.

and Faraday rotators which were originally used in the Orion laser can be used to amplify the single-mode laser radiation.

Narrow linewidth is necessary for high-resolution nonlinear optical experiments which provide data (such as Raman linewidths) necessary for accurate CARS measurements. A pulse-amplified ring dye system with a linewidth of approximately 0.01 cm^{-1} will be used in conjunction with the single-mode Nd:YAG laser to perform high-resolution Raman spectroscopy. The argon-pumped ring dye laser will be installed later this year and will be pulse-amplified with the aid of Nd:Yag-pumped dye cell amplifiers.

DIANA LASER BEAM CHARACTERIZATION

D. A. Stephenson, C. B. Layne

Diana, a flashlamp-pumped dye laser, is one of two central lasers specifically designed for combustion science experiments carried out in the Combustion Research Facility. Diana's output consists of 1-2 microsecond pulses at up to 10 Hz, the wavelength dependent upon the dye selected and capable of covering the visible spectrum. The output is directed on demand to any of the facility laboratories by means of a periscope beam-distribution system.

The amount of usable laser energy from Diana available in remote laboratories is determined by the mechanical stability of the periscope, the optical quality of the gas in the laser duct, the mirror losses, and the laser beam divergence. Previous experiments have verified that the mechanical stability of the periscopes is excellent and does not significantly degrade the beam quality. On the other hand, beam motion due to index-of- refraction gradients inside the laser ducts has been measured. To alleviate problems caused by air drafts, the ducts were sealed more effectively and changes are being made to the air-conditioning equipment. Since mirror losses are controlled by modern dielectric coatings, which provide greater than 99 percent reflectivity over broad spectral ranges in the visible, beam divergence remains as the limiting factor.

A new energy diagnostic in Diana measures the energy into a given divergence angle (typically 1.5 mr) by focusing a fraction of the final output through a pinhole and onto a photodiode. The divergence angle subtended by the photodiode is fixed by the lens focal length (0.5 m) and the pinhole diameter (0.75 mm). The photodiode signal is thus representative of deliverable energy and is used to optimize alignment and amplifier energy settings.

A series of measurements of deliverable energy from Diana were made by placing calorimeters in Diana and in a remote laboratory with a light path of 30 m. With coumarin 440 dye (producing laser light at 440 nm), the energy loss was 11 percent at low pump energy and 32 percent at intermediate and high pump energies. The total energy reached was 0.1 J in Diana. With coumarin 504 dye (producing laser light at 530 nm), the losses were 22 percent at low pump energy and 35 percent at high pump energy (2.3 J in Diana). Energies of 7 J are possible in Diana, but higher losses were also observed. (Some fraction of these losses is due to scattering from dirty mirrors in the periscopes, a problem that will be solved by continuously purging the laser ducts with clean air.)

The reticon array, near-field—far-field camera described in a following article was used to characterize Diana's oscillator beam divergence for the two laser dyes currently in use. The divergence with coumarin 504, the best high-energy blue-green dye, is 1.1 ± 0.1 mr (milliradian) at normal pump energy. This value increases slightly to 1.2 ± 0.2 mr for coumarin 440, which is a blue dye with lower output energy but significantly shorter wavelength (440 nm). The increased pump energy required for lasing with coumarin 440 probably accounts for the slight increase in divergence. Output is less reproducible with coumarin 440, since the oscillator operates closer to threshold.

The beam in the Diana system increases in diameter by a factor of three as it propagates through the amplifiers and the final beam-expanding telescope. This effect would reduce the beam divergence by a factor of three if all the optical elements were perfect. In fact, however, the final beam divergence is approximately 1.5 mr, the exact amount depending on pump energies and alignment. Passive (unpumped) optical distortion in the first amplifier is easy to observe when one sends an HeNe laser through the dye tube. The initially collimated beam focuses about 3 m beyond the amplifier. To the extent that this distortion approximates a simple lens, it is corrected by an adjustable telescope between the oscillator and first amplifier (and again by the final telescope). It is important to characterize the distortion and its dependence on dye flow rate, dye solvent, and flow geometry. Similar, though less serious, distortions are apparent in the final two amplifiers. Control of these sources of beam divergence may significantly increase the usable output from Diana.

A series of measurements have been made to characterize the flow-induced focusing problem in Diana's amplifiers. This focusing is most pronounced in the first amplifier, which is 8 mm in diameter. Initial experiments ruled out any bending of the windows on the dye cuvette; so the only credible source of the focusing appears to be temperature-induced index variations. It is interesting to note that the observed focusing of about 0.25 diopter can be explained by a density gradient of only 2 ppm from the center to the outside of the tube. For water as the dye solvent, this value implies a temperature gradient of 0.004 K. For an equal mixture of water and methanol the gradient would only be 0.0014 K. The flow through the dye cuvettes is intentionally turbulent to ensure thorough mixing of the dye and so prevent such small temperature gradients. To determine the origin of these relatively small gradients, we carefully measured the temperature of the dye tubing at various points along the flow path. We found a temperature increase of about 0.1 K per elbow in the dye pipe, whether the dye was warmer or cooler than the environment. This initially startling observation can be understood from a simple conservation of energy calculation, which predicts a temperature rise of 0.002 K per psi of pressure drop for water. This is the temperature that the bulk of the fluid will have after complete mixing, but of course most of the energy is generated at the walls; so the fluid there is initially hotter.

We were able to reduce the focusing in the 8 mm amplifier by replacing the somewhat complicated collection of sharp bends in the steel pipe with a sweeping plastic pipe. It is likely that the reduction could be improved even further by a better design of the inlet fitting. Even if the plumbing were perfect, however, there would still be a pressure drop and some heating from friction with the walls of the dye cuvette itself. A calculation shows that a pressure drop of about 5 psi is required to clear the dye sample between laser shots. This lower limit on the heat input will create different index variations in different fluids. A solution of 10 percent methanol in water was used to test these ideas. The resulting laser performance was very poor, but the passive focusing of the 8 mm amplifier was again reduced by a factor of two. This effect occurred because water has a higher heat capacity and a lower change of index with temperature than does methanol. An important goal of our work is to find the optimum dye-solvent mixture having good thermal properties and good lasing characteristics.

THE FACILITY COMPUTERS

D. E. Benthusen

Computing equipment at the Combustion Research Facility includes a remote job entry terminal (RJET) to allow sophisticated modeling jobs to have access to computers in Sandia's central computing facility (CDC 6600s, VAXes, and a CRAY-1), a VAX11/780 super-mini computer for software development and data reduction, and a number of PDP11s and small VAXes which control laboratory experiments. Some of the latter computers are able to transfer data to the VAX11/780 by means of DECNET.

The RJET currently consists of a card reader, a line-printer, and a control terminal which attaches directly to one of the CDC 6600s; and jobs can be staged from there to the CRAY if desired. The RJET presently in use will be replaced with a VAX11/730, which will support disks and mag tape in addition to performing all the present RJET functions. The RJET area also has four additional terminals that can access the computers located in the central computing facility.

A wealth of graphics software is now available to VAX users. The ISSCO DISSPLA can be used to produce plots on a variety of output devices such as the Tektronix 4014, Versatec, and Printronix printer-plotters. Also, TELL-A-GRAF and CUECHART (ISSCO) have been added to the VAX repertoire. These are graphics systems that accept plain English commands and can display input data in the form of a plot, a bar-chart, or a pie-chart. In addition, a Sandia-designed program called TEXT is very useful for making high-quality viewgraphs. All of these systems are now capable of producing graphics in color when used in conjunction with an appropriate output device. The above-mentioned products have been integrated into a Sandia-designed software system called the "Virtual Graphics Device" (VGD). The VGD features a very compact metafile, powerful graphics editing, and the capability to write files that can be processed directly on the Dicomed Computer Output Microfilm system to produce journal-quality output.

Since this graphics software would be useless without the proper output devices, we are in the process of building a graphics work station. The station contains a low-resolution graphics terminal with color monitor that can be used for graphics program development, an eight-color pen plotter capable of producing high-quality output on opaque backgrounds, and a combination high-resolution color graphics terminal and camera capable of doing extensive graphics editing and producing either slides or viewgraphs of the results.

New additions to the VAX software have continued to increase its usefulness in the area of text processing. An office automation package called "All-In-One" provides word-processing, filing, and desk management capabilities. Another word processor called MUSE provides capabilities matching those provided by stand-alone word processors. Improved software has been developed to support the letter-quality printers which are used to produce correspondence, reports, and similar material. This software can produce printed output using only 10 percent of the CPU time required by the previous system. We have also upgraded the TEX typesetting software so that it has not only increased functionality but runs more efficiently on the VAX as well.

Several hardware additions have also been made to the VAX this year. The configuration had consisted of the CPU, four megabytes of memory, one nine-track 800-1600 BPI mag-tape drive, three RP06 and two RP07 disk drives (1.73 gigabytes total capacity), four printer-plotters, 96 terminal I/O ports, which support five Tektronix graphics terminals, and sixty-five terminals of various other types, as well as printers and plotters used for text generation. To this we have added a pair of 6250 BPI mag-tape drives, a port contender which will allow as many as 256 terminals in the terminal network, and approximately 30 additional terminals.

Examination of the VAX accounting files and the Sandia-implemented performance monitoring software indicates that the use of the CRF VAX has been increasing steadily. Our data indicate that we are using 65-70 percent of the available cpu time during any given month. The connect time indicates an average of 36-40 users on the machine during all the working hours in the month. While it is certain that some of this connect time was logged after normal working hours, the peak user load has been reaching 40-45 on most afternoons. The performance monitoring data also shows that, while 65-70 percent cpu use does not occur every day, there are many times when the average over the day is in the 95-100 percent range. These figures indicate that we could increase the computing done on the VAX by encouraging users to run jobs (batch) at night and on weekends. However, there are also a number of factors acting to increase the peak interactive demand on the VAX, and the necessary capability to meet these demands must be provided.

DATA REDUCTION

Mathematical manipulation of experimental data has been one of the intended uses for the VAX, and the machine has been used extensively for data reduction and the subsequent plotting of the reduced data by means of the DISSPLA graphics software. Now that DECNET is a reality, there are three experiments that will be sending large quantities of data to the VAX for reduction. As more laboratories are completed and especially as the facility is expanded, this activity will increase manyfold.

GRAPHICS

In addition to the DISSPLA graphics software, which is used extensively to plot both experimentally obtained and theoretically derived data, there are three additional graphics packages, TEXT, TELL-A-GRAF, and CUE-CHART, which are being used interactively by an increasing number of staff. More sophisticated 3-D graphics, such as the Evans-Sutherland picture system, are also available but will require an increase in our computing power to make them practical.

TEXT GENERATION

Text generation and processing continues to be a significant activity on the VAX. Text generation (i.e. the use of text editors) does not greatly impact the system because it meshes well with other jobs and, in fact, uses only cpu cycles that would have gone unused anyway. On the other hand, text processors, such as RUNOFF or TEX, place significant demand on the processor and tend to slow down other work being done on the system. It is clear that these processors—especially TEX—are growing in popularity; thus we must either limit their use administratively or provide more cpu power to support them.

To support growth in the foregoing activities, it will be necessary to increase the computing capability at the CRF. This end can be accomplished in two phases; and if the upgrades are applied in the time-frames described below, CRF computing needs will be adequately served through FY-88 and beyond.

The first upgrade should take place late in FY-83 or early FY-84 It would consist of adding a second processor which would be devoted entirely to text-oriented activities. If the processor is to support only the CRF text activities it could be a VAX11/750; however, if we were to provide support for the text processing done by other organizations, then the machine would have to be a VAX11/780. In any case, both of these VAXes would be connected to a network (a computer interconnect), which also serves as an interface between the two CPUs and would have a common file system (disks). This configuration (known as a cluster) has twice the compute power of our single VAX, still has a single file system, allows execution of currently running programs without any modification, allows easy file sharing among users on the two different CPUs, and allows users to have access to all of their files, regardless of which machine being used. Even though we intend to keep the scientific processing on one CPU and the text processing on the other, it would be possible to cross these lines in an emergency; so neither the scientific processing nor the text processing would have to come to a halt in the event of a CPU failure.

The second stage of the upgrade can take place any time in FY-85 or early FY-86. By then, we expect several manufacturers to be offering minicomputers with the capability of roughly three-quarters of a CDC-7600. One of these machines would augment the VAX-CLUSTER; and, compatability permitting, it seems likely that such a maxi-mini would become part of the cluster. This arrangement would create a system of multiple cpu's (the computer interconnect can support up to 14), all using the same file system. This capability would readily support the increased data reduction, graphics, and text processing loads that are anticipated.

The PDP 11s are being added as needed to control laboratory experiments through the CAMAC or other specially designed interfaces. These minis use the RT 11 operating system; and Fortran is the primary applications-level language, although interpretive languages are available for those whose needs are better served by an interactive language. There are currently twenty three PDP11s in operation to control laboratory experiments; however, we are finding that the current capabilities of the laboratory minicomputers (such as the PDP11/34) directly coupled to experiments are no longer adequate to meet the increased demands for both memory and processing speed which are imposed by applications such as two-dimensional imaging. Array processors with additional memory attached to existing PDP11s provide a cost-effective way to provide the necessary capability. There is reason to expect that this improved capacity would allow us to take more and larger data arrays or images and to process them in a much shorter time. This, in turn, makes it practical to consider more sophisticated data processing than is presently possible. However, while we expect that an array processor will do those things (they are normal array processor functions), it has yet to be demonstrated that the combination computer and processor can function as a real-time image processor. To evaluate the feasibility in a prototype system, we are now acquiring such a processor. Also this year, we have purchased a VAX11/730 to control one of the facility lasers. This is our first attempt at real-time control using a virtual memory machine and we expect a number of challenges in the area of locking-down code so that it doesn't swap out just when it is needed.

VISITING SCIENTIST PROGRAM

R. H. Johnsen

The Visiting Scientist Program enables scientists from universities, industry, and other national laboratories to take advantage of the special equipment and resources available at the Combustion Research Facility by doing research here. So long as the visitor is willing to make the results of such research generally available, preferably in published form, there is no cost imposed for the project. Research support provided to visiting scientists includes technicians and engineering staff dedicated to the project, computer time, shop work, and other purchases used in direct support of the project. The visitor generally provides whatever salary, travel, and living expenses are necessary. Proprietary research can also be done here, but it must be arranged on a full-cost-recovery basis.

Since the facility opened early in 1981, we have had more than 1600 technical visits. Nearly 1300 of these visits were brief, typically for one or two days. These short-term visitors generally came here either to learn something about what we do or to discuss specific problems of their own in combustion research with members of our staff.

About 300 of the visitors spent from three to five days here and usually were involved in more detailed discussions on some particular aspect of combustion research. Many of them attended either a short course or a workshop held here at the facility.

The list of visiting scientists spending up to a month or more at the CRF, now exceeds 50. Those visiting in 1982-83 (listed below) have engaged in a wide variety of research projects and have included representatives from universities, industry, and other national laboratories. Commencing in 1982, we have also had graduate students here doing thesis work under the guidance of a faculty advisor and a mentor assigned from the Sandia staff.

Visitors are free to execute their own research projects or they can arrange to work in collaboration with members of the facility staff. To date, our visitors have elected primarily to work on collaborative projects or to use some pre-existing experimental setup to do their own research.

SHORT COURSES

R. H. Johnsen

As a special category of educational effort, we periodically offer short courses at the Combustion Research Facility. They are generally focused on transferring to interested attendees advanced technology developed here. Wherever possible, these courses include laboratory sessions closely coupled with the formal lectures.

In June 1982, for example, the course dealt with "Optical Diagnostics in Internal Combustion Engines" and consisted of two and one-half days of lectures, coupled with one and one-half days of practical laboratory sessions. The laboratory experiments included

- Using LDV to measure in-cylinder fluid motion

- Using optical pyrometry to measure particulate temperature and density in a constant-volume bomb

- Using coherent anti-Stokes raman spectroscopy to measure temperature in a homogeneous-charge engine

- Applying spontaneous Raman scattering for measurements in a homogeneous-charge engine

- Flow visualization techniques in an internal-combustion engine

Distinguished outside lecturers for the course included Charles A. Amann, General Motors Corporation; Prof. Frediano V. Bracco, Princeton University; Dr. Antonio D'Alessio, CNR Laboratorio de Ricerche sulla

VISITING SCIENTISTS—1982-83

Visitor	Affiliation	Term of Stay	Project
P. Ariessohn	Weyerhaeuser	7/83	High-Temperature Particle Mass Detector Research
M. Azzazy	Spectron Dev Lab	2/83	Species in Flames
R. Blint	General Motors	4/82	Flame Modeling
C. Borgnakke	U Michigan	6/82-8/82 7/83-8/83	Turbulent Flames Modeling in Engines
T. Bowman	Stanford U	9/82-3/83	Soot Formation
M. Branch	U Colorado	2/83-8/83	Ammonia Chemistry
N. Brown	LBL	11/80-Open	NH3 Kinetics
L. Cloutman	LANL	9/81-9/82	Engine Modeling
M. Colket	UTRC	1/83	Premixed Laminar Flame Measurements
J. Craig	Spectron Dev Lab	2/83	Species in Flames
G. Dobbs	UTRC	1/83	Premixed Laminar Flame Measurements
H. Dwyer	UC Davis	6/74-Open	Combustion Modeling
C. Escoda**	Yale U	1/82-2/82	Flame Ramanography
D. Fourguette**	Yale U	1/82-2/82 6/82-8/82	Flame Ramanography
M. Frisch	Carnegie-Mellon U	7/83	Theoretical Studies of Bond Energies
N. Henein	Wayne State U	4/83-5/83	Diesel Alternative Fuels
E. Hurt**	Louisiana State U	6/83-12/83	Laser Induced Fluorescence
W. Kollmann	U C Davis	7/81-Open	Turbulence Modeling
N. Laurendeau	Purdue U	6/-83-7/83	Coal Combustion
M. Long	Yale U	1/82-2-82 6/82-8/82	Flame Ramanography
J. Martin**	U Michigan	6/82-8/82	Turbulent Flames Modeling in Engines
		1/83-5/84	Turbulent Flame Measurement
R. Mendez	Naval Postgrad	6/83-8/83	Vortex Dynamic Methods
S. Medina*	San Jose State U	6/83-8/83	Engine Combustion Lab Asst
R. Nichols	Spectron	2/83	Species in Flames
G. Patniak**	Carnegie-Mellon U	6/83-8/83	Combustion Modeling
N. Peters	RWTH Aachen	9/83-10/83	Turbulence Modeling
D. Pines*	U New Hampshire	6/83-8/83	Chemical Kinetics Lab Asst
S. Rajan	So Ill U	6/81-8/81 6/82-7/82	Turbulence in Premixed Flames
D. Ruzicka	LBL/Central Inst Research, Norway	12/82-7/83	Alternate Fuels Diesel Combustion
K. Saito	Toshiba Corp	9/83-9/84	Pulsed Combustor Measurements
S. Schneider	Westinghouse R&D	6/82-12/82	CARS/Fluorescence Detection
E. Slamovich**	LBL	6/83	Particle Size Measurement
A. Smith	U Manchester	5/82-6/82	Computational Modeling
L. Thomas	Chem Dynamics	8/81-4/82	Collision Theory
S. Vosen	U C Berkeley	8/83-6/84	Unsteady Flame Propagation
G. Voth	Cal Inst Tech	6/83	Vibrational Spectra Calculations
D. Wardlaw	Cal Inst Tech	6/83	Vibrational Spectra Calculations
J. Warnatz	Heidelberg U	3/82-9/82	Computational Flame Chemistry/Diagnostics

*Undergraduate Student

** Graduate Student

Combustion, Naples, Italy; and Prof. W. C. Reynolds, Stanford University. Members of the Sandia research staff also gave lectures, and they conducted all of the laboratory sessions.

There were 66 people registered for the course. Because of the heavy enrollment and the limited capacity in the laboratory sessions, one-third of those registered (many of them students from nearby universities) attended lecture sessions only. The total group included representatives from government agencies and laboratories, universities and national laboratories, and industry. Fifteen of those attending were from countries other than the U. S., including Canada, Norway, the United Kingdom, Germany, Sweden, Italy, and Japan. Several of those attending from U. S. universities were also non-U. S. citizens. All together, there were thirteen countries represented at this short course.

These courses and workshops covering various phases of our work are offered from time to time at the Combustion Research Facility. They constitute an important step in fulfilling our charter to transfer as expeditiously as possible to the combustion community at large information, techniques, and instrumentation developed here.

10.0 Stanford Linear Accelerator Center
Stanford Synchrotron Radiation Laboratory (SSRL)

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

Answer: The new science being explored at SSRL is all related to the unique x-ray, soft x-ray and vacuum ultra-violet radiation provided by the Laboratory. In the x-ray region, the intense, tunable radiation is used to determine atomic arrangements in complex systems in which such arrangements could not be determined previously, using the extended x-ray absorption fine structure and anomalous scattering of x-rays. Examples of such studies are: determinations of the changes of surroundings of important metal atoms in metalloenzymes and metalloproteins as these materials undergo their biological functions, as well as determinations of atomic arrangements in polyatomic glasses, alloys, and amorphous thin films. These techniques are also utilized to determine atomic arrangements on the surfaces of materials so as to understand phenomena such as rusting, other corrosion and the poisoning of catalysts. The structural procedures being developed here also allow for the determination of atomic arrangements in surface layers of amorphous materials. No other technique exists for this purpose.

The x-rays are also being used to develop the technique of non-invasive angiography. The goal of this work is to eliminate the need for the dangerous catheterization procedure required to locate blockages of heart arteries prior to by-pass operations. The approach being followed will also decrease markedly the dose of x-rays used for such diagnosis and eliminate expensive hospitalizations.

The soft x-rays are being used to develop x-ray lithography for eventual use in the production of very large scale integrated circuits. Related techniques are being used to develop x-ray microscopy for the study of both biological and inorganic materials.

The soft x-rays are also used, via EXAFS techniques (extended x-ray absorption fine structure, a method of locating atoms' neighbors), to determine atomic arrangements around light atoms such as phosphorus, sulfur, aluminum, and silicon.

The vacuum ultraviolet (VUV) radiation is used to study the electronic and structural properties of metal and semiconductor surfaces as well as interfaces on an atomic scale. Such knowledge is also employed for the development of very large integrated circuits as well as catalysis.

The VUV is also employed to study fundamental photoionization processes in gases and solids. Such knowledge is quite broadly applied in atomic, molecular, solid state and plasma physics as well as astrophysics.

Finally, the VUV is employed for the characterization of semiconductor materials (defects in devices, structure, etc.).

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

   Answer: SSRL is presently the only facility in the United States which runs in a dedicated mode for the production of x-ray synchrotron radiation. While other rings operate at lower energies for the production of soft x-ray and VUV radiation in a dedicated mode, none do yet for the production of harder x-rays. This situation will change when the 2.5 GeV ring of the National Synchrotron Light Source at Brookhaven becomes operative. Until then, however, all of SSRL's x-ray facilities are unique.

   In addition, SSRL presently has 3 x-ray wiggler lines and one soft x-ray undulator line which are expected to remain unique until at least 1985 when their capabilities will be matched by similar devices at NSLS.

   SSRL is presently undertaking the development of an x-ray undulator line on the 14-GeV storage ring PEP. That line will remain unique for the indefinite future.

   In the soft x-ray machine, SSRL's monochromator, JUMBO, which serves the 800 to 4000 eV range and is completely ultrahigh vacuum, is unique and will be until its capabilities are duplicated at Aladdin in Wisconsin or NSLS.

   The time structure of SSRL is unique. That is, it provides 200 picosecond (trillionths) wide pulses every 780 nanoseconds (billionths).

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

   Answer: SSRL presently has 18 experimental stations covering the energy range 1 - 45000 eV. Six of these stations cover the VUV and soft x-ray portion of the spectrum. The remainder address the hard x-ray portion. The most powerful line is expected to radiate 1.6 kW when fully commissioned in the near future. In addition to the beam lines, which are fully equipped with monochromators, experimental hutches, and the necessary end station electronics, a variety of specialized instrumentation is available. This instrumentation includes: a two-circle, a four-circle and a six-circle diffractometer; an ultra-high vacuum sample chamber; an area detector for protein crystallography; a rotation camera facility for protein crystallography; a soft x-ray undulator; an insertion device; a scattering camera; a biochemical preparation laboratory; and a VAX 11/780 for data processing.

   The attached brochure "General Information and Proposal Guidelines" specifically describes the characteristics of each experimental station and item of specialized instrumentation. On page 3, the standard end station equipment provided to users is detailed.

STANFORD SYNCHROTRON RADIATION LABORATORY

GENERAL INFORMATION
AND
PROPOSAL GUIDELINES

MARCH 1984

STANFORD SYNCHROTRON RADIATION LABORATORY

PROPOSAL GUIDELINES

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P.O. Box 4349, Bin 69
Stanford, CA 94305

SSRL SHIPPING ADDRESS
BLDG. 120
2575 Sand Hill Road
Menlo Park, CA 94025

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SSRL PROPOSAL SUBMITTAL FORM

USER AGREEMENT APPLICATION FORM

THE SSRL FACILITY

SSRL is a national facility supported by the Department of Energy and the National Institutes of Health for the utilization of synchrotron radiation for research in the natural sciences and engineering. It is a user-oriented facility which welcomes proposals for experiments from all qualified scientists.

The synchrotron radiation is produced by the 4 GeV storage ring, SPEAR, operated by the Stanford Linear Accelerator Center (SLAC) under a contract with the Department of Energy.

Section I of this booklet details the guidelines for the writing and submission of proposals, explains the procedures used to review and rate proposals and the manner in which experiments are scheduled for beam time. Section II gives general information for users. Section III describes the characteristics of the SSRL experimental stations and specialized instrumentation.

Another booklet entitled "Users Information Guide" is available from the facility and contains practical information for SSRL user (lists of motels, rental cars agencies, the telephone system, stores supplies, etc.) An annual Activity Report covering facility developments and user science is also available.

SECTION I: PROCEDURES FOR PROPOSAL SUBMISSION, PROPOSAL RATING AND BEAM TIME ASSIGNMENT

I-A. PROPOSAL SUBMISSION

Proposals for experimental work at SSRL are accepted at any time. However, due to the length of the reviewing process, deadlines of September 1 and March 1 of each year are established for consideration at the following January or June Proposal Review Panel meeting. Proposals received after these deadlines will not be guaranteed consideration at the next PRP meeting.

Proposals are considered for single experiments and for experimental programs. Proposals for single experiments are considered active for two years after their initial rating by the Proposal Review Panel. Program proposals may be renewed once after two years at the discretion of the Proposal Review Panel based on evidence of satisfactory progress as demonstrated by the Activity Report.

Although most of the proposals active at SSRL are for experimental work aimed at producing significant new scientific results, SSRL also welcomes proposals for testing and development of scientific instrumentation, particularly when these instruments are likely to have impact on synchrotron radiation research.

PROGRAM PROPOSALS: A program proposal should be a series of experiments with a single unifying intellectual theme. The proposal, however, should be divided into identifiable segments to aid in assessing progress. The various parts of the proposal should be related closely enough to be reviewable by a single expert in the field. A proposal will not be considered as a program unless it requires at least 25 shifts with 50 to 100 shifts being the expected norm.

I-A.1. REQUIRED FORMAT AND CONTENTS OF PROPOSALS

Proposals must contain a Proposal Submittal Form (attached at end of booklet) and written text in the following prescribed format. A USER AGREEMENT APPLICATION FORM for each funding source represented in the proposal must be submitted simulanteously. See SECTION II-B.

A. Description of Experiment
B. Experimental Equipment
C. Equipment Development Schedule
D. Previous Experience with the Technique and Facility
E. Safety Concerns
F. End Station and Beam Time Requirements
G. Resources for Program Proposals (program proposals only)

Proposals which do not follow this format will not be sent out for refereeing until correctly amended. Proposals should be between 3-10 pages in length.

Fifteen (15) double-sided copies of each proposal, typed single space or space and a half, should be submitted to Katherine Cantwell, SSRL. Each proposal should be accompanied by the appropriate User Agreement application forms (attached at end of booklet).

Upon receiving a proposal, an acknowledgment is sent to the Spokesperson. If you do not receive such acknowledgment within two weeks of submitting your proposal contact Carol Mitchell at SSRL.

DETAILS OF PROPOSAL CONTENTS

The Proposal Submission Form is at the end of this booklet. It must be completely filled out and copies attached to each copy of the proposal. The Spokesperson indicated on this form is responsible for all communications with SSRL staff (i.e. scheduling, special equipment needs, characteristics of samples, and in particular, safety requirements). **The designated Spokesperson should be the person who will actually be responsible for these matters.**

SECTION A. Description of Experiment

In this section give a description of the subject matter of the proposal. This description should include a statement of its scientific purpose, the reason synchrotron radiation is needed, the theoretical background, samples to be used, procedures to be followed, previous experimental results, and, if known, a comparison of competing, or closely related experiments planned or in progress at other facilities.

If a proposal is being submitted as a replacement for an expiring proposal it should include explicit and easily found information about past beam usage and reports. That is, information should be included on the number of shifts used, the energy, the experimental station used and other relevant information, and references to all publications and reports.

SECTION B. Experimental Equipment

In this section list the major facility equipment to be used and the space and services required for the experiment. SSRL has available for experimental use a variety of detectors, computers, and other specialized equipment and also provides electrical, water, air, gaseous helium and liquid nitrogen services. Standard equipment to be found on an x-ray station includes: small (1) and large (1) ionization chambers, exit slits (1), sample positioner (1), Keithly 427 current-to-voltage amplifier (2), Anadex voltage-to-frequency converter (3 channels), Hewlett-Packard x-y recorder (1), Fluke high voltage power supply (1), Kinetic Systems hex scaler (1), Kinetic Systems up-down presettable counter (1), Ortec real-time clock (1), Joerger stepping motor controller (2), Borer PDP 11/CAMAC crate controller (1), Standard Engineering Corporation CAMAC Power Supply (1), PDP 11 computer and peripherals (usually an 11/34) (1) Kinetic Systems D to A converter. Contact Teresa Porter at the Facility for more information. Specialized equipment must be itemized on the Beam Time Request Form.

SECTION C. Equipment Development Schedule

In this section give an estimate of the date when the equipment to be supplied by the experimenter will be ready for installation.

For experiments on the SSRL vacuum beam lines, details of the equipment and samples to be used are required at least 3 months before the experiment is to be run. In order to maintain performance levels of beam lines, and the storage ring itself, experiments on the vacuum lines are carefully examined to assure the designs emphasize reliability and conform to ultra-high vacuum practice, and that risks of contamination are avoided. A list of acceptable sample materials and high vacuum devices, fabrication and cleaning techniques, etc., is available upon request from SSRL. All materials not on this list must be tested and approved by SSRL prior to use.

Consultation with facility staff is essential at an early stage when planning new equipment for connection to vacuum beam lines. Persons planning such experiments who are unfamiliar with SSRL/SPEAR experiment fabrication requirements should write to SSRL and request **SLAC-TN-73-13** (SSRL User Specifications for Vacuum Systems and Components which Interface with the SPEAR Vacuum System).

SECTION D. Previous Experience with the Techniques and Facility

To aid reviewers and the PRP in their assessment of the prospects for successful completion of the experiment and its analysis, the proposers should provide a brief description of their previous experience with the techniques and equipment they expect to use at SSRL. When appropriate, this information may be provided in the form of list of publications on experimental work related to that performed at SSRL. Familiarity with the facility and previous successful use is a relevant factor in judging proposals. If work has not been previously done in this area, a general description of the scientific background and publications of the principal collaborators should be included.

SECTION E. Safety Concerns

All experiments performed at SSRL must conform to the SLAC and SSRL safety standards. It is the responsibility of the Spokesperson to develop procedures for dealing with potentially hazardous situations.

Section E of the proposal must contain either the following statement:

> **No hazardous material, equipment, or procedure will be brought to SSRL as part of this proposed experiment.**

or must contain:

1. A list of all hazardous materials, including quantity and morphology.
2. A list of recommended safety procedures designed to ensure a safe, healthful environment while at SSRL.
3. A description of any hazardous equipment or procedure and recommended safety precautions.

A hazardous material is anything that is ignitable, corrosive, reactive or toxic (including radioactive).

Prior approval is required before any of the above may be brought to SSRL. The approval process is achieved by:

1. Completing the steps above.
2. Providing a Material Safety Data Sheet (MSDS) for all hazardous materials you intend to bring.
3. Receiving a numbered Safety Review Print-out (see next paragraph).
4. Submitting the Print-out with your verification of its accuracy attached to your Beam Time Request Form.

All proposals are reviewed for safety concerns by the SSRL staff. The spokesperson is notified if the proposal raises any specific concerns. **Proposals with unresolved safety concerns are not eligible for beam time.** Please remember that experiments at SSRL are performed in an often crowded experimental floor in close proximity to other experiments. Thus, procedures which may be reasonable in a small laboratory occuppied by a few people all of whom are familiar with the possible hazards, may not be acceptable at SSRL.

Before being permitted to work at SSRL all experimenters must read the SSRL Safety Guidelines and sign a User Safety Agreement indicating that they understand and will conform to these guidelines. In addition each new user receives a safety orientation from the Operations Manager. It is the responsibility of the spokesperson to make sure that members of the experimental group have signed a User Safety Agreement before they actually begin working on the SSRL experimental floor.

SMOKING IS NOT PERMITTED ON THE EXPERIMENTAL FLOOR.

RADIOACTIVE MATERIALS: SSRL maintains a modest supply of weak radioactive sources. These sources will be loaned to experimenters for use at SSRL on request. The user is responsible for keeping track of the source and returning it to the SSRL operator. We encourage experimenters to use sources available at SSRL and avoid bringing sources to the project from outside labs. If you must bring your own special source to SSRL please list it in the Safety Section of your proposal.

SECTION F. Experimental Station and Beam Time Requirements

Experimental Station Requirements - State clearly the preferred experimental station(s) and give all possible alternatives. If there are no alternatives, state why. For a description of the characteristics of SSRL experimental stations consult Section III of these guidelines.

Beam Time Requirements - Show clearly the basis for estimating the amount of beam time required. You may include a reasonable contingency factor for failures and adjustments of the detection equipment, but you should not allow a contingency for failure of the accelerator or the beam system leading up to your apparatus. Please indicated if it is possible to perform any or all of your experiment under parasitic conditions.

Figure 1 is the basic spectral distribution curve of SPEAR for both the wiggler and bending magnets. This curve can be used as a starting point in estimating the flux expected. This curve gives the raw theoretical photon flux produced by SPEAR, integrated over the full vertical angular opening of the beam. It is uncorrected for absorption in Be windows, He path, mirror and crystal reflectivity, etc. It has been generally found that, after all attenuation corrections have been made, the useful flux is still below that expected from the curves - in some cases, by a factor of ten or more. It is advisable to consult with SSRL staff or other experimenters about actual flux that may be expected on a given station under the condition of a given experiment.

SECTION G. Resources for Program Proposals

(Include only if submitting a program proposal.) In this section clearly outline the manpower, equipment, and financial resources available to you to carry out this program to completion in order to demonstrate to the referees and PRP that such a program can be accomplished.

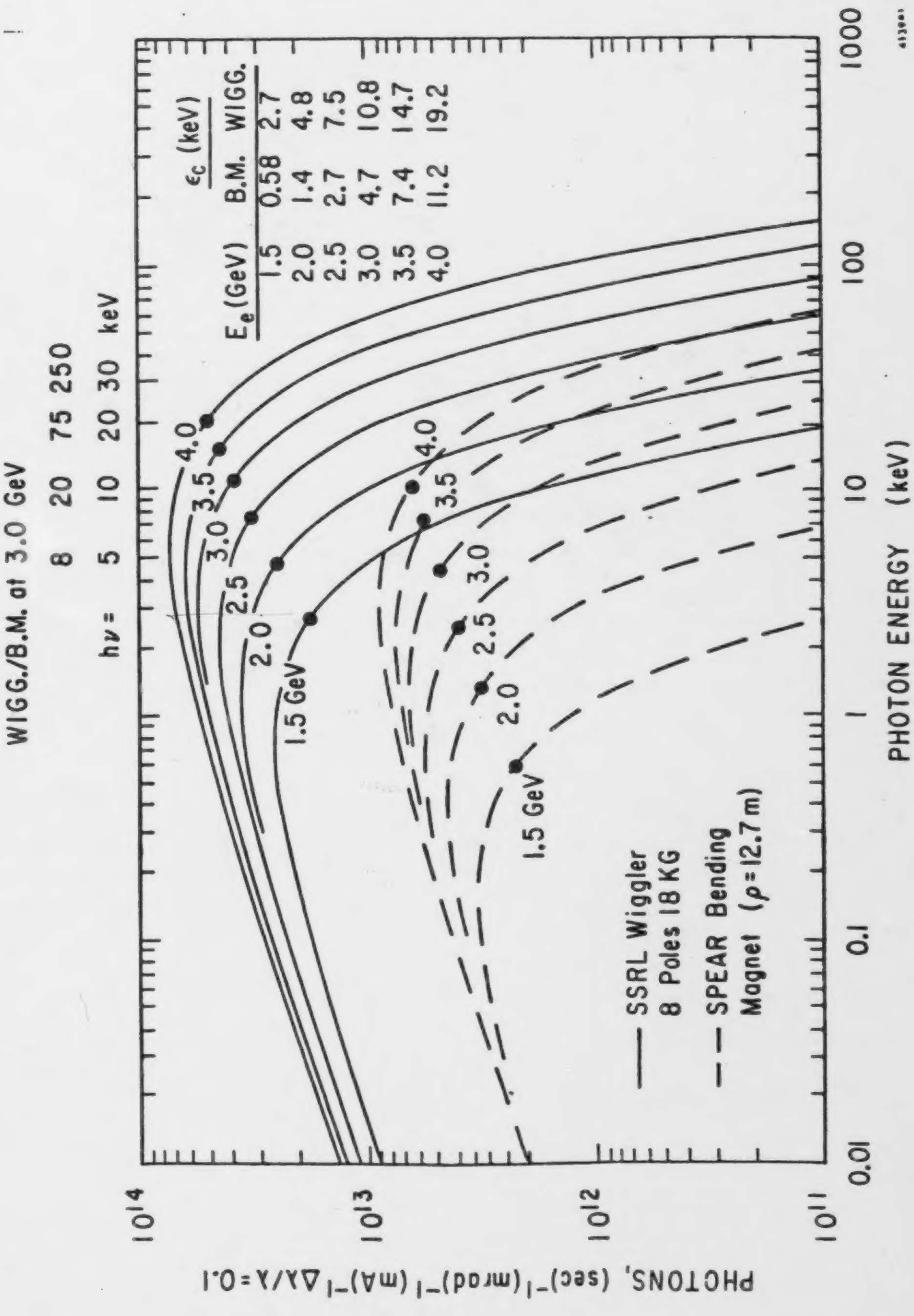
WIGG./B.M. at 3.0 GeV
hν = 5 8 20 75 250 keV
2 5 10 20 30
E_e (GeV) | B.M. | WIGG.
ε_c (keV)
1.5 0.58 2.7
2.0 1.4 4.8
2.5 2.7 7.5
3.0 4.7 10.8
3.5 7.4 14.7
4.0 11.2 19.2
4.0
3.5
3.0
2.5
2.0
1.5 GeV
4.0
3.5
3.0
2.5
2.0
1.5 GeV
SSRL Wiggler 8 Poles 18 KG
SPEAR Bending Magnet (ρ = 12.7 m)
10^14
10^13
10^12
10^11
PHOTONS, (sec)^-1 (mrad)^-1 (mA)^-1 Δλ/λ = 0.1
0.01
0.1
1
10
100
1000
PHOTON ENERGY (keV)

FIGURE 1

I-A.2 LETTERS OF INTENT

Beam time may be assigned on the basis of a letter of intent under a limited set of conditions. A letter of intent may be submitted to SSRL for one of two purposes: to test the feasibility of a "risky" experiment or, for a new user group, to obtain the experience necessary to write a full-scale proposal. Letters of intent do not go through the full review process but may receive a single assignment of a small amount of beam time at the Director's discretion or on the advice of the Proposal Review Panel. In general, rated proposals take priority over Letters of Intent in the scheduling process.

A letter of intent should briefly address the problem to be examined, the amount of time and beam energy required, the beam station required, and the time frame within which the test is desired. Letters of Intent must specifically state whether or not the content is proprietary. These letters of intent should be addressed to Katherine Cantwell, Assistant to the Director. Letters of intent must specifically state whether or not they include proprietary research.

I-A.3 PROPRIETARY RESEARCH

Stanford University's policy guidelines on secrecy in research must be followed in performing proprietary research at SSRL. In accordance with these guidelines classified research cannot be performed at the Facility. Proprietary Research by SSRL Users may be permitted at SSRL under the following guidelines:

(a) Proprietary research is to be separately identified and proposed to the Director of SSRL as either Proprietary Research Proposals or as Proprietary Research Letters of Intent.

(b) Proprietary Research Proposals are to be competitively reviewed (including referee reviews) for scientific merit in accordance with standard SSRL policies and procedures. Proprietary Research Letters of Intent are to be competitively reviewed by the SSRL Proposal Review Panel for scientific merit.

(c) Proprietary research is to be scheduled in accordance with standard SSRL policies and procedures.

(d) Although Stanford will not accept any institutional responsibility for protecting the confidentiality of any material identified as proprietary in proprietary research proposals, it will, through the Confidential Conferee (as defined below) and not inconsistent with its contractual obligations to the Government utilize reasonable efforts to protect the confidentiality of the User's specifically identified proprietary information.

(e) No proprietary research is to be conducted on a beam line during any Users' priority time utilization of that beam line.

(f) User is expected to mark each piece of proprietary data with an appropriate legend.

(g) The SSRL Director is to identify an SSRL Confidential Conferee to monitor the proprietary research performed.

(h) During the time proprietary information is being maintained in confidence, the Confidential Conferee is to not serve as a confidential conferee or enter into consulting arrangements with others concerning technology directly related to the subject matter of the proprietary research without the prior written consent of the User.

(i) The User is to provide the Confidential Conferee with the necessary information as requested by the Confidential Conferee, including proprietary data, which will be subject to the 90-day period described below, concerning the materials and details of the experiment, prior to the allocation of beam time. Short interim progress reports may be required of the User during the investigation and data processing of proprietary information.

(j) User is to make available generally all intellectually significant results of the experimental work at SSRL not later than the end of the 90-day period described below. The preferred form of disclosure of such results would be an article submitted for journal publication. Other forms could be considered subject to the mutual agreement of the User and SSRL.

(k) The aforesaid period of 90 days is to be the 90-day period immediately following completion of the analysis of data which is shown to be a substantial completion of the problem(s) stated in the proprietary research proposal. After conferring with the User concerning determination of the starting date of the 90-day period, the Confidential Conferee is to establish and notify the User in writing promptly of the determined starting date.

(l) The Confidential Conferee is to make reasonable efforts to maintain all proprietary data and confidential discussions in confidence and not make them part of the public SSRL record or otherwise part of the public domain until the expiration of the 90-day period described above, or until made available generally by the User, whichever comes first. In the former case, the Confidential Conferee is to make the proprietary information a part of the public SSRL record.

(m) The User is to pay, on the basis of full cost recovery, facility charges for use of the facilities of SSRL, including a beam time charge for that portion of the work on samples whose identity the User requests be maintained confidential. Facility charges are not to be levied for auxiliary measurements on standard materials unless the User requests that such information be maintained in confidence. Facility charges should be specified as a dollar amount per hour of beam time and such charge rate should be provided to the User prior to commencement of the experiments described in the User's proprietary research proposal.

(n) The User's institution is to sign an SSRL User Agreement and an SSRL Supplemental User Agreement for each individual proprietary research proposal undertaken.

I-B. PROPOSAL REVIEW PROCESS

Upon receipt of a correctly formatted proposal it is sent to the Proposal Review Panel members whose fields of expertise are closest to the subject matter of the proposal. These panel members suggest appropriate referees for the proposal. Referee suggestions may also be made by the proposal spokesperson and by other referees. In this manner, two to six written referee reports are obtained for each proposal. These reports, with referee's names deleted, are sent to the spokesperson as they are received. The Proposal Review Panel convenes twice a year in January and June. At this meeting the panel members review the referee reports and other materials relevant to the new proposals and assign a rating between 1.0 (highest) and 5.0 (lowest) for each proposal.

The Proposal Review Panel - The Panel consists of ten scientists with expertise in various research fields using synchrotron radiation. For the purpose of rating proposals the panel is divided into three sub-panels. The current members of the panel and their sub-panels are as follows:

X-ray Absorption and Scattering in Biological Systems

Charles Cantor, Columbia University, Chair
Wayne Hendrickson, Naval Research Laboratories
William Orme-Johnson, MIT

Vacuum Ultra-Violet and Surface Science

Bernd Crasemann, University of Oregon
Charles Fadley, University of Hawaii
Warren Grobman, IBM, Yorktown Heights

X-ray Absorption and Scattering in Materials

Bob Batterman, Cornell University
Denis McWhan, Bell Laboratoires
David Turnbull, Harvard University
Hutch Harnsberger, Harnsberger Associates

In addition to determining ratings the Proposal Review Panel advises on policy concerning scheduling and proposal processing as well as more general matters affecting the user community.

I-B.1 APPEALS TO PROPOSAL REVIEW PANEL RATINGS

Ratings assigned by the Proposal Review Panel may be appealed on the basis of the specific grounds listed below. Except in extraordinary circumstances appeals will be dealt with at the following meeting of the PRP. Appeals must be received at SSRL 6 weeks BEFORE the panel meeting in question. Appeals should be addressed to Katherine Cantwell.

The grounds for appeals are:

1. The PRP did not receive a spokesperson's response to one or more reviews.

2. There is a significant discrepancy between the reviewer's comments and the PRP ratings, and the remarks supplied by the PRP with their ratings are not a sufficient explanation of that discrepancy.

3. Appeals of previously rated proposals may be made based on unanticipated experimental results or new instrumentation development since the initial rating.

I-C. SCHEDULING PROCEDURES

SSRL operates as a dedicated synchrotron radiation source for fifty percent of the SPEAR operating time. The remainder of the time SSRL operates parasitically during colliding-beam runs for the SLAC high energy physics program.

Beam Time Request Forms are sent to spokespersons for all active proposals in advance of each run. Experimenters are requested to fill out these forms stating their needs. These needs are then matched with the energy schedule and beam time is assigned in accordance with the ratings received from the PRP.

Changes to the SPEAR schedule can occur due to unanticipated problems with the storage ring or the linear accelerator. Since these changes can occur on very short notice they may result in the cancellation of an already scheduled experiment. In most cases, short-term adjustments to the SSRL schedule cannot be made to compensate for unusually poor performance of the storage ring or problems with the equipment.

Two additional factors which may enter into the determination of the schedule are:

1. The Director of SSRL may grant priority time for a limited period to individuals who, or institutions which, have contributed significantly to the development of facility instrumentation.

2. The Director of SSRL may schedule small amounts of beam time for special purposes at his discretion.

SECTION II. GENERAL INFORMATION FOR USERS OF THE SSRL FACILITY

II-A. USER PURCHASE ORDERS AND ACCOUNTS

There are no costs associated with use of non-proprietary SSRL beam time which are charged to the user, and, except as described in Section II-E, there are no charges for services provided by the SSRL staff. Also, there is no charge for use by experimenters (with approval of SSRL staff, of a small machine shop equipped with lathe, milling machine, drill press, etc. Experimenters are urged to bring their own small tools, marked and in a lockable box. **However**, experience has shown that most users require materials and/or services (including SLAC computer time) that must be purchased through SLAC or other parts of Stanford.

To bear experimental costs that are not covered by SSRL before commencing experiments, the user must issue to Stanford University a check to establish an advance funded account. This check should be for the estimated amount of expenditure but must be for at least $500.00. Any unexpended balance will be refunded. Checks should be sent to M. Stickler, Accountant SSRL. Further information regarding procedures for establishing this fund can be obtained from Marsha Stickler (extension 3456).

II-B. SSRL USER AGREEMENT

Stanford, in order to comply with its contractual agreements with the Department of Energy (DoE), as well as its own insurance policies, requires that all experiments (based on proposals or letters of intent) at SSRL shall be under the terms and conditions of a User Agreement signed by both the user's institution and Stanford. A user agreement must be executed by each institution working at SSRL for each funding source within that institution. **A form to apply for a User Agreement is found at the end of this booklet and must be submitted with each proposal for each funding source represented in the Proposal.** Copies of the relevant Patent Rights Clause and Rights in Data and Copyright Clause must be attached to these forms. Further information can be obtained by contacting Katherine Cantwell, ext. 3191.

II-C. PAPERS BASED ON WORK AT SSRL & REQUIRED ACKNOWLEDGMENT

We annually publish a list of all user publications for distribution to the user community and interested parties (SSRL Report 80/04). Please send notices of articles published and theses completed to Carol Mitchell. Publication information is of particular interest to our funding agencies.

All abstracts, reports and publications should acknowledge research work done at the Facility with the following sentence on the title or first page:

> "The work reported herein was (partially) done at SSRL which is supported by the Department of Energy, Office of Basic Energy Sciences; and the National Institutes of Health, Biotechnology Resource Program, Division of Research Resources."
>
> VUV proposals may drop the reference to the NIH. If work was done before November 1982 the following NSF reference should be inserted: "National Science Foundation, Division of Materials Research".

II-D. SHIPPING EQUIPMENT, STORAGE AND WORKSPACE AT SSRL

Storage space and workspace at SSRL is very limited. Experimenters requiring workspace beyond the small work areas at each experimental station must make arrangements with SSRL Operations staff (Chuck Troxel) for specific work space two weeks before the start of the run.

Neither SLAC nor SSRL are contractually responsible for shipping or receiving users' equipment; however, we can and will facilitate these activities. Please examine your User Agreement for a description of Stanford's general liability.

All equipment brought in for a run SHOULD ARRIVE NO SOONER THAN ONE WEEK PRIOR TO YOUR ARRIVAL and must be removed at the end of each assigned block of time unless storage space has been assigned by an SSRL Operations staff member. Prior to completion of your experiment, please make shipping arrangements with Linda Crum.

Equipment being shipped to SSRL should clearly be marked "Property of (Your Institution)". To aid in locating your shipment, mail a copy of your shipping document (with Air or Way Bill Number) to Linda Crum on the day the shipment leaves your institution. The label and shipping document should include your name, c/o Linda Crum, in order to expedite the shipment through SLAC receiving. All communication with SLAC Shipping and Receiving should be through Linda Crum.

The SSRL shipping address is:

Your name c/o Linda Crum
SSRL
SLAC, Building 120
2575 Sand Hill Road
Menlo Park, CA 94025

PLEASE REMEMBER DUE TO LACK OF STORAGE SPACE YOUR SHIPMENT SHOULD NOT ARRIVE MORE THAN A WEEK IN ADVANCE OF YOUR ARRIVAL.

If special experimental equipment is to be brought to SSRL from a foreign country, please contact Linda Crum for assistance prior to shipment. To cover the costs of customs clearance, shipment from SF International Airport, etc. you must first open an advanced funded user account at SSRL.

II-E. SUPPORT SERVICES PROVIDED BY SSRL TECHNICAL STAFF

The SSRL technical staff can supply only incidental services to experimental groups free of charge. These incidental services include limited assistance with experimental installation, and electrical and mechanical work in connection with installing an experiment. Because of the impact on the availability of SSRL staff for general user support, complex installation jobs involving major modifications of facility or user equipment for a specific experiment, and major mechanical or electrical fabrication jobs, will generally be sent to SLAC shops or performed at SSRL by SLAC technicians brought in for this purpose. The actual charges involved will be billed to the user's account.

In the case of jobs which (for radiation safety or personnel or vacuum protection reasons) have to be done directly by SSRL staff, adequate notice (two-to-three months) should be given to minimize their impact on running periods where demands on staff time are at their peak. Because of the impact of such major jobs on other staff duties, labor and material costs for these jobs will be charged to user accounts even though performed by SSRL staff unless they are of general benefit to the user community.

Floppy disks and mag tapes are available at SSRL for retention by users; they will be charged to your account. See Sharon Spillane to obtain.

II-F. COMPUTER FACILITY USAGE

There are three facets to computer usage at SSRL:

Beam Line Computers
Media Transfer Facilities
Central VAX System Computer Facility.

Beam Line Computers: Nearly all the beam lines have 11/34 computers with a VT100 console terminal and RL01 disk drives. If you need something different this must be noted on your Beam Time Request Form.

The Beam Time Request Form should also indicate which operating system (RSX-11M V4.0 or RT-11 V4) and which SSRL supported software, if any, you wish to use. All further developments in software will be using the RSX operating system. Thus users are encouraged to use the RSX data acquisition packages. If you want a graphics terminal (both VT125 and an old model Selanar graphics VT100 are available in limited quantities), indicate this also. The RSX EXAFS programs currently use the Selanar graphics.

Media Transfer Facilities: There is an 11/34 front end processor on the VAX system which is used mostly for DECnet and media transfer. On this system one can transfer RSX Files-11 files between RX01, RL01, RK05, and 800 BPI magtape. There is also a command procedure to copy RT-11 files from RL01 or RX01 to magtape in either ANSI or DOS format. There is a description posted in the VAX terminal room. In addition there is a computer in the x-ray group lab that can transfer files from RL01 to magtape under RT-11. In order to get RT-11 ANSI tapes from RX01, arrangements must be made with Seth Goldberg. This is also true for transfers from RL02 to other media.

The VAX room 11/34 is also the system one uses to transfer files on and off the VAX system using DECnet. There is a short description of how to do this in the VAX terminal room. However, Seth Goldberg or Ann Waldhauer should be contacted before doing this for the first time.

Vax Computer Facility: A VAX 11/780 with 2.5Mb memory, a floating point accelerator and a fixed media RA81 drive is available for on-site use only for preliminary analysis of data taken at SSRL.

Users can bring in their own analysis routines and use the VAX to analyze data taken here. See Seth Goldberg to make arrangements for this service. The only compliers on the VAX are FORTRAN-77 and Whitesmith's C. Most programs written in standard FORTRAN will recomplie and run easily on the VAX.

Tony Cox has installed a documented analysis package on the VAX for use with data taken from the RSX EXAFS data acquisition package. The program uses VT125 graphics and hardcopy is obtained from the Versatec on the 11/34 in the VAX terminal room.

You will need an account for any extensive use of the VAX. See Seth Goldberg for acquiring one. There are usually 6 VAX terminals available (most with VT125 graphics) in a terminal room outside the VAX room. There are limited other lines near some beam lines. See Seth Goldberg for details and note desire on beam time request form.

Data is not to be kept permanently on the public user pack and programs may be archived until the user's next visit. Data can be transferred to the VAX via DECnet from the 11/34 in the VAX room and in some cases from beam line computers running RSX. See Seth Goldberg for details and note desire on beam time request form.

II-G. BIOCHEMICAL LABORATORY USAGE

A biochemical and chemical laboratory is available for users. It is under the supervision of Axel Golde. If you plan to use this facility it should be noted on your Beam Time Request Form. The laboratory includes: an ultracentrifuge, a scanning uv-vis spectrophotometer, a milligram balance, a stereo-microscope, a hydraulic cell press, and an inert atmosphere box. Support facilities include a millipore deionized water system (which provides 18 megohm water), an ice maker, a refrigerator-freezer, a laboratory glassware washer, and a large cold box for chromatography.

II-H. MEMBERS OF THE SSRL STAFF

The following is a partial list of the SSRL staff whom users most generally need to contact. You are encouraged to contact the appropriate member of the SSRL staff regarding any questions you may have. Inquiries of a general nature should be addressed to Katherine Cantwell, Assistant to the Director (x 3191), who will then route your inquiry to the person most capable of handling it.

SSRL PHONE NUMBER (415) 854-3300 FTS 461-9300

For information on the characteristics, capabilities and performance of SSRL branch lines and instrumentation, please contact the SSRL staff scientist listed below. Documentation on most branch lines and systems is available through Katherine Cantwell.

Branch Line I-1	Piero Pianetta	x 2874
Branch Line I-2	Piero Pianetta	x 2874
Branch Line I-4	William Warburton	x 2874
Branch Line I-5	George Brown	x 2092
Branch Line II-2	George Brown	x 2092
Branch Line II-3	George Brown	x 2092
Branch Line II-4	George Brown	x 2092
Branch Line III-1	Piero Pianetta	x 2874
Branch Line III-3	Piero Pianetta	x 2874
Branch Line III-4	Piero Pianetta	x 2874
Branch Line IV-2	George Brown	x 2092
Branch Line IV-3	William Warburton	x 2874
Branch Line VII-2	George Brown	x 2092
Branch Line VII-3	George Brown	x 2092

Area Detector System	Paul Phizackerley	x 2874
Biotech/Chemical Laboratory	Axel Golde	x 2091
CAD-4 Detector	Paul Phizackerley	x 2874
Huber Diffractometer	George Brown	x 2092
VAX Computer	Seth Goldberg	x 2874
VG Sample Chamber	Piero Pianetta	x 2874
Scattering Camera	Steve Hubbard	497-2479
Rotation Camera	Paul Phizackerley	x 2874

For information on experimental support, please contact the following members of the technical staff:

SPEAR Running Parameters	John Cerino	x 2874
Safety Concerns & Hazards	John Cerino	x 2874
Gas & Cryogenics Orders	Chuck Troxel	x 2896
Electrical Equipment Needs	John Yang	x 2896
Vacuum Equipment Needs	Harry Morales	x 2896
Other Equipment Needs	Sharon Spillane	x 2896

For information on administrative matters; please contact the following members of the administrative staff:

Accounting	Marsha Stickler	x 2033
Purchasing	Linda Crum	x 2066
Dosimeters	Michelle Steger	x 2874
Overseas Shipments	Linda Crum	x 2066
Proposal Submittal	Katherine Cantwell	x 3191
Scheduling	Katherine Cantwell	x 3191
SSRL Reports	Carol Mitchell	x 2874
User Agreements	Katherine Cantwell	x 3191
User Publications	Carol Mitchell	x 2874

SECTION III: CHARACTERISTICS OF SSRL EXPERIMENTAL STATIONS AND SPECIALIZED INSTRUMENTATION

SSRL presently has 17 experimental stations in operation. These provide white radiation and monochromatic radiation over a broad spectral region from the visible through the ultraviolet and deep into the x-ray region to 40 KeV and beyond. The characteristics of these stations and specialized instrumentation available to users are briefly summarized in the following section. Further information on the experimental stations may be obtained from the responsible SSRL staff scientist listed above. Documentation on the various experimental stations may be obtained by contacting Katherine Cantwell.

EXPERIMENTAL STATION I-1 (4°)

RESPONSIBLE SCIENTIST	PIERO PIANETTA
FOCUSING MIRROR:	2° ANGLE OF INCIDENCE, Au or Pt COATING
MONOCHROMATOR:	GRASSHOPPER: GRAZING INCIDENCE
A) SLITS:	FIXED ENTRANCE AND EXIT SLITS 10 μm
B) GRATING(S):	2 M CONCAVE REFLECTION GRATING Au or Pt COATED BLANK SIZE: 35 x 45 x 10 mm RULED AREA: 25 x 35 mm TYPICAL RULINGS: 300-2400 ℓ/mm
PHOTON ENERGY:	300 ℓ/mm: hν > 16 eV 600 ℓ/mm: hν > 32 eV 1200 ℓ/mm: hν > 64 eV 2400 ℓ/mm: hν > 128 eV UPPER LIMIT: ∿ 1000 eV
ENERGY RESOLUTION: ΔE	$\Delta E = 8 \times 10^{-5} \Delta\lambda (h\nu)^2$ where: ΔE (eV) hν (eV) Δλ (A) Δλ = 0.4 A 300 ℓ/mm Δλ = 0.2 A 600 ℓ/mm Δλ = 0.1 A 1200 ℓ/mm Δλ = 0.05 A 2400 ℓ/mm
PHOTON FLUX AT SAMPLE:	$(1-10) \times 10^{7}$ Photons/Sec/mA
SPOT SIZE:	1 x 2 mm
INSTRUMENTATION:	COMPUTER: PDP 11/34 CPU (SHARED WITH STATION I-2) TEKTRONIX 4025 TERMINAL TEKTRONIX HARD COPY UNIT CAMAC CRATE: HEX SCALER REAL TIME CLOCK D/A CONVERTER STEPPING MOTOR CONTROLLERS UP-DOWN COUNTER NIM ELECTRONICS: V/F CONVERTER LINEAR AMPLIFIER

LEVEL ADAPTER
DISCRIMINATOR
5 kV HV SUPPLY
RATEMETER

RESEARCH: ULTRA-HIGH VACUUM COMPATIBLE EXPERIMENTS

STATUS: OPERATIONAL

EXPERIMENTAL STATION I-2 (8°)

RESPONSIBLE SCIENTIST: PIERO PIANETTA

MIRRORS:

M$_o$: 30 x 5 cm PLANE, Pt-COATED COPPER
4° GRAZING INCIDENCE

M$_1$: 22.9 x 12.7 cm CYLINDRICAL
Pt-COATED QUARTZ,
3.3 m RADIUS OF CURVATURE
(HORIZONTAL FOCUSING 17.5° INCIDENCE)

M$_2$: 10.2 x 5.1 cm CYLINDRICAL
Pt-COATED QUARTZ, 4.48 m
RADIUS OF CURVATURE
(VERTICAL FOCUSING NEAR NORMAL
INCIDENCE)

M$_3$: REFOCUSING MIRROR

MONOCHROMATOR: 1 m SEYA-NAMIOKA, 70.25° BETWEEN INCOMING AND OUTGOING BEAMS

A) SLITS: 1 mm, 0.2 mm, 0.1 mm, 0.02 mm

B) GRATINGS:

1200 ℓ/mm (300 A blaze) Os coated
1200 ℓ/mm (1500 A blaze) Os coated
1200 ℓ/mm (600 A blaze) Os coated
1180 ℓ/mm (1500 A blaze) Al/MgF$_2$ coated
590 ℓ/mm (5000 A blaze) Al/MgF$_2$ coated

ILLUMINATED AREA ON GRATING 30 x 15 mm^2

PHOTON ENERGY RANGE: 4 - 40 eV

ENERGY RESOLUTION: 0.2 - 6.0 A

PHOTON FLUX AT SAMPLE: (1-10) x 10^8 PHOTONS/SEC/mA

SPOT SIZE: Approximately 1 X 3 mm^2

FILTERS: QUARTZ, LiF, In, Sn

INSTRUMENTATION:

COMPUTER: PDP
11/34 CPU (SHARED WITH STATION I-1)
TEKTRONIX 4025 TERMINAL
TEKTRONIX HARDCOPY UNIT
CAMAC CRATE:
HEX SCALER
REAL TIME CLOCK
D/A CONVERTER
STEPPING MOTOR CONTROLLERS

	UP/DOWN COUNTER NIM ELECTRONICS: V/F CONVERTER LINEAR AMPLIFIER LEVEL ADAPTER DISCRIMINATOR 5 kV HV SUPPLY RATEMETER
RESEARCH:	ULTRA HIGH VACUUM COMPATIBLE EXPERIMENTS GAS PHASE EXPERIMENTS BELOW 11.6 eV (LiF WINDOW CUT-OFF)
STATUS:	OPERATIONAL

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EXPERIMENTAL STATION I-4

RESPONSIBLE SCIENTIST: WILLIAM WARBURTON

MIRROR: FLOAT GLASS, ELLIPTICAL, UNCOATED, 10 to 1 DEMAGNIFYING

MONOCHROMATOR: Si(111), CURVED AND ASSYMETRICALLY CUT

ENERGY RANGE: 6,000 eV - 9,500 eV

ENERGY RESOLUTION: 60 eV at 8.7 KeV FOR ASSYMETRICALLY CUT CRYSTAL.

HORIZONTAL ANGULAR ACCEPTANCE: 2.2 MRAD

SPOT SIZE: 0.25 mm VERTICAL x 0.5 mm HORIZONTAL

ABSORPTION:
525 micron Be
4 M He
35 micron C

MEASURED FLUX: Approximately 1.6 x 10^{10} PHOTONS/SEC AT 1.73 A, SPEAR AT 3.0 GeV, 55 mA

INSTRUMENTATION:
DECTECTOR
RETICON LINEAR PHOTODIODE ARRAY, 1024 ELEMENTS .001" x .100", COUPLED TO PHOSPOR BY FIBER OPTICS
NIM ELECTRONICS
DETECTOR SPECIFIC ELECTRONICS, PLUS H.V. SUPPLY, AMP/TSCA, RATEMETER, PM I_o DETECTOR
CAMAC ELECTRONICS
12 BIT DAC, 16K DUAL PORT MEMORY, HEX SCALER, DATAWAY DISPLAY, UP-DOWN COUNTER, GPIB INTERFACE, QUAD INPUT AND OUTPUT REGISTERS, DUAL POWER SUPPLY CONTROL, 12 BIT A/D CONVERTER, BORER 1533B CONTROLLER
COMPUTER
PDP 11/05, 32 K BYTE, DUAL FLOPPY DISC DRIVE, PAPERTAPE READER, LA36 TERMINAL, OUTPUT TO TEKTRONIX VARIABLE PERSISTANCE DISPLAY
STEPPER MOTOR CONTROL
32 MOTOR MULTIPLEXED CONTROLLER

STATUS: OPERATIONAL

RESEARCH: SMALL-ANGLE X-RAY SCATTERING

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EXPERIMENTAL STATION I-5 (EXAFS I)

RESPONSIBLE SCIENTIST:	GEORGE BROWN
MIRROR:	NONE
MONOCHROMATOR:	Si(220) Si(111), Parallel Crystal Geometry DOWNWARD REFLECTING
ENERGY RANGE:	2,800 eV - 30,000 eV
HORIZONTAL ANGULAR ACCEPTANCE:	1.0 MRAD
SPOT SIZE:	1-3 mm VERTICAL 20 mm HORIZONTAL
ABSORPTION:	533 micron Be 10 M He 35 micron C
INSTRUMENTATION:	PDP11/34 CPU, VT100 Terminal RL01 DISC DRIVE, MAGTAPE DRIVE CAMAC CRATE HEX SCALER REAL TIME CLOCK STEPPING MOTOR CONTROLLERS UP-DOWN COUNTER V-F CONVERTERS (3) ION CHAMBERS (2) PREAMPLIFIERS (2) DIGITAL TO ANALOG CONVERTER
STATUS:	OPERATIONAL
RESEARCH:	EXAFS, EDGE ABSORPTION SPECTROSCOPY, ATOMIC SCATTERING

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EXPERIMENTAL STATION II-2

RESPONSIBLE SCIENTIST	GEORGE BROWN
MIRROR:	Bent cylinder, fused quartz, platinum coated. Radii: 1500 m (adjustable) x 10 cm Mean grazing incidence: 8.8 mrad Cut-off energy: 8.9 KeV Magnification: 1.0 Adjustable Horizontal Slit Upstream of Mirror Removable
MONOCHROMATOR:	Si(111), Si(220) PARALLEL CRYSTAL GEOMETRY UPWARD REFLECTING
ENERGY RANGE:	2,800 - 8,900 eV FOCUSED.
HORIZONTAL ANGULAR ACCEPTANCE:	0-4.8 MRAD
SPOT SIZE:	1 mm x 4 mm
ABSORPTION:	533 micron Be 15.5 m He 35 micron C
INSTRUMENTATION:	CAD-IV 4-CIRCLE DIFFRACTOMETER, PDP 11/34 CPU, VT100 TERMINAL, RL01 DISC DRIVES, CAMAC CRATE, HEX SCALER, REAL TIME CLOCK, STEPPING MOTOR CONTROLLERS, UP-DOWN COUNTERS, V-F CONVERTERS (3), ION CHAMBERS (3), PREAMPLIFIERS (2), DIGITAL TO ANALOG CONVERTER
STATUS:	OPERATIONAL
RESEARCH:	PROTEIN CRYSTALLOGRAPHY, SURFACE EXAFS, SMALL-ANGLE SCATTERING

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EXPERIMENTAL STATION II-3

RESPONSIBLE SCIENTIST:	GEORGE BROWN
MIRROR:	NONE
MONOCHROMATOR: GEOMETRY	Si (111), Si (220), PARALLEL CRYSTAL
ENERGY RANGE:	2,800 - 30,000 eV
HORIZONTAL ANGULAR ACCEPTANCE:	1.0 MRAD HORIZONTAL
SPOT SIZE:	5 mm x 20 mm
ABSORPTION:	533 micron Be 13.5 M He 35 micron C
INSTRUMENTATION:	PDP 11/10 CPU, LA 36 TERMINAL, RX01 FLOPPY DISC DRIVE, CAMAC CRATE, HEX SCALER, REAL TIME CLOCK, STEPPING MOTOR CONTROLLERS, UP-DOWN COUNTERS, V-F CONVERTERS (3), ION CHAMBERS (2), PREAMPLIFIERS (2), DIGITAL TO ANALOG CONVERTER*
STATUS:	OPERATIONAL
RESEARCH:	DILUTE EXAFS, X-RAY FLUORESCENCE SPECTROSCOPY

*A new PDP 11/34 CPU, VT100 Terminal, RL01 disc dirve and tape drive are scheduled for installation in March 1984.

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EXPERIMENTAL STATION II-4

RESPONSIBLE SCIENTIST:	GEORGE BROWN
MIRROR:	NONE
MONOCHROMATOR:	NONE - WHITE RADIATION
HORIZONTAL ANGULAR ACCEPTANCE:	1.0 MRAD
SPOT SIZE:	1.5 mm x 17 mm
ABSORPTION:	533 micron Be 10 M He 35 micron C
INSTRUMENTATION:	NONE
STATUS:	OPERATIONAL
RESEARCH:	X-RAY TOPOGRAPHY

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EXPERIMENTAL STATION III-1

RESPONSIBLE SCIENTIST:	PIERO PIANETTA
FOCUSING MIRROR:	2° ANGLE OF INCIDENCE Au COATED
MONOCHROMATOR:	GRASSHOPPER: GRAZING INCIDENCE
A) SLITS:	IN SITU ADJUSTABLE ENTRANCE AND EXIT SLITS $10\,\mu$m < WIDTH < 200 m
B) GRATING(S):	TWO 2 m CONCAVE REFLECTION GRATINGS IN SITU INTERCHANGEABLE Au or Pt COATED BLANK SIZE: 20 x 37 x 8 mm RULED AREA: 13 x 34 mm TYPICAL RULINGS: 300-2400 ℓ/mm
PHOTON ENERGY RANGE:	300 ℓ/mm: $h\nu > 16$ eV 600 ℓ/mm: $h\nu > 32$ eV 1200 ℓ/mm: $h\nu > 64$ eV 2400 ℓ/mm: $h\nu > 128$ eV UPPER LIMIT: ∿ 800 eV
ENERGY RESOLUTION: ΔE	$\Delta E = 8 \times 10^{-5}\, \Delta\lambda (h\nu)^2$ where: ΔE (eV) hν (eV) Δλ (A) with 10 m slits: Δλ = 0.4 A 300 ℓ/mm Δλ = 0.2 A 600 ℓ/mm Δλ = 0.1 A 1200 ℓ/mm Δλ = 0.05A 2400 ℓ/mm
PHOTON FLUX AT SAMPLE:	$(1-10) \times 10^7$ PHOTONS/SEC/mA WITH $10\,\mu$m SLITS
SPOT SIZE:	1 X 1 mm
INSTRUMENTATION:	COMPUTER: PDP 11/34 CPU VT100/Selamar GraphicsLA120/Selamar Graphics

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EXPERIMENTAL STATION III-1 (Continued)

	CAMAC CRATE: HEX SCALER REAL TIME CLOCK D/A CONVERTER STEPPING MOTOR CONTROLLERS UP-DOWN COUNTER
	NIM ELECTRONICS: V/F CONVERTER LINEAR AMPLIFIER LEVEL ADAPTER DISCRIMINATOR 5 kV HV SUPPLY RATEMETER
RESEARCH:	ULTRA HIGH VACUUM COMPATIBLE EXPERIMENTS
STATUS:	OPERATIONAL

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EXPERIMENTAL STATION III-2 (WINDOWLESS BRANCH LINE)

MIRRORS:	FIVE EXOTICALLY FIGURED MIRRORS WITH ANGLES OF INCIDENCE LARGER THAN 79°
MONOCROMATOR:	GRAZING INCIDENCE CERNY-TURNER MONOCHROMATOR WITH A 1200 ℓ/MM PLANE GRATING.
ENERGY:	5 eV to 160 eV (2480 A - 75 A) POLARIZATION: 98% AT 10 eV AND > 96% AT 160 eV
RESOLUTION:	FOR FULL APERATURE AT ENTRANCE SLIT $1\text{-}2 \times 10^3$ (E/ΔE)
ANGULAR ACCEPTANCE:	HORIZONTAL ACCEPTANCE 8 MRAD
SPOT SIZE:	ONE-HALF SPEAR SOURCE (1.6 mm HORIZONTAL x .3 mm VERTICAL AT 3 GeV)
OUTPUT FLUX:	TO BE DETERMINED
INSTRUMENTATION:	DIFFERENTIAL PUMPING SYSTEM TO ENABLE EXPERIMENTAL CHAMBER TO OPERATE AT A TOTAL PRESSURE OF 10^{-3} TORR
STATUS:	IN CONSTRUCTION STAGE
RESEARCH:	GAS PHASE AS WELL AS UHV EXPERIMENTS

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EXPERIMENTAL STATION III-3 (CRYSTAL MONOCHROMATOR/JUMBO)

RESPONSIBLE SCIENTIST:	PIERO PIANETTA
MIRROR:	FUSED QUARTZ, BENT CYLINDER PLATINUM COATED, MEAN GRAZING ANGLE 17 MRAD MAGNIFICATION 1.0
MONOCHROMATOR:	PARALLEL DOUBLE CRYSTAL GEOMETRY 4 IN SITU INTERCHANGEABLE CRYSTALS FIXED EXIT BEAM
ENERGY RESOLUTION:	0.35-0.8 eV (FWHM) FOR hν = 800-1550 eV (Beryl 10$\bar{1}$0) 0.25-0.35 eV (FWHM) FOR hν = 1500-1800 eV (Quartz (10$\bar{1}$0) 1.5-7.0 eV (FWHM) FOR hν = 1800-4000 eV (InSb(111)) 1.0-2.0 eV (FWHM) FOR hν = 1900-4000 eV (Ge(111))
ENERGY RANGE:	800-4000 eV
HORIZONTAL ANGULAR ACCEPTANCE:	10 MRAD
SPOT SIZE:	2 mm x 4 mm
ABSORPTION:	NONE, VACUUM PATH, OR FILTERS (SILICON, CARBON, ALUMINUM)
INSTRUMENTATION:	PDP 11/34 CPU VT100/Selamar Graphics LA120/Selamar Graphics

CAMAC CRATE:
- HEX SCALER
- REAL TIME CLOCK
- D/A CONVERTER
- STEPPING MOTOR CONTROLLERS
- UP DOWN COUNTER

NIM ELECTRONICS:
- V/F CONVERTER
- LINEAR AMPLIFIER
- LEVEL ADAPTER
- DISCRIMINATOR
- 5 kV HV SUPPLY
- RATEMETER

MONO OUTPUT FLUX MONITOR:
- GRID (SILVER, COPPER, NICKEL)
- CHANNELTRON
- BATTERY BOX
- CURRENT TO VOLTAGE AMPLIFIER

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RESEARCH:	ULTRA-HIGH VACUUM COMPATIBLE, NON ULTRA-HIGH VACUUM SEPARATED BY THIN WINDOW
STATUS:	OPERATIONAL

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EXPERIMENTAL STATION III-4 (3°)

RESPONSIBLE SCIENTIST:	PIERO PIANETTA
MIRROR:	QUARTZ, TORODIAL, PLATINUM COATED
MONOCHROMATOR: .	GENERAL PURPOSE, COMPATIBLE WITH BRAGG DIFFRACTION ELEMENTS, GRATINGS, & ZONE PLATES. UNDER DEVELOPMENT.
ENERGY RANGE:	0 - 3000 eV
ENERGY RESOLUTION:	WHITE RADIATION OR VARIOUS TYPES OF MONOCHROMATOR ELEMENTS POSSIBLE.
HORIZONTAL ANGULAR ACCEPTANCE:	0.6 MRAD
SPOT SIZE:	ABOUT 2 mm x 8 mm
ABSORPTION:	NONE, VACUUM PATH
INSTRUMENTATION:	DIFFERENTIAL PUMPING SYSTEM (SAMPLE CHAMBER 10^{-7} TORR)
STATUS:	DEVELOPMENTAL TESTING AND LIMITED OPERATION.
RESEARCH:	LITHOGRAPHY/MICROSCOPY; GRATING AND ZONE PLATE TESTING

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EXPERIMENTAL STATIONS IV-2 & VII-2 (Wiggler End Stations)

RESPONSIBLE SCIENTIST:	GEORGE BROWN
MIRROR:	BENT CYLINDER, FUSED QUARTZ, PLATINUM COATED RADII: 1500 M (ADJUSTABLE) X 10 CM MEAN ANGLE OF INCIDENCE: 7.7 MRAD, CUT-OFF
CUT-OFF	ENERGY: 10.2 KeV MAGNIFICATION: 1.0 REMOVABLE
MONOCHROMATOR:	TWO-CRYSTAL, Si(111), Si(220) UPWARD REFLECTING
ENERGY RANGE:	2,800 to 10,200 eV WITH MIRROR 2,800 to 50,000 eV WITHOUT MIRROR
HORIZONTAL ANGULAR ACCEPTANCE:	0 - 4.6 MRAD WITH MIRROR 1 MRAD WITHOUT MIRROR
SPOT SIZE:	2 mm x 5 mm WITH MIRROR 5 mm x 20 mm WITHOUT MIRROR
ABSORPTION:	533 micron Be 1 M He 35 micron C
INSTRUMENTATION:	PDP 11/34 CPU, VT 100 TERMINAL RL01 DISC DRIVES CAMAC CRATE HEX SCALER REAL TIME CLOCK STEPPING MOTOR CONTROLLERS UP-DOWN COUNTERS V-F CONVERTERS (3) ION CHAMBERS (2) PREAMPLIFIERS (2) DIGITAL TO ANALOG CONVERTER
STATUS:	OPERATIONAL
RESEARCH:	EVERYTHING

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EXPERIMENTAL STATIONS IV-1, IV-3 & VII-3 (WIGGLER SIDE STATIONS

RESPONSIBLE SCIENTIST:	GEORGE BROWN
MIRROR:	NONE
MONOCHROMATOR:	PARALLEL CRYSTAL Si (111), Si (220) DOWNWARD REFLECTING
ENERGY RANGE:	2,800 eV - 50,000 eV
HORIZONTAL ANGULAR RESOLUTION:	1.0 MRAD
SPOT SIZE:	1.5 mm x 19 mm
ABSORPTION:	533 micron Be 1 M He 35 micron C
INSTRUMENTATION:	PDP 11/34 CPU, VT 100 TERMINAL RL01 DISC DRIVES CAMAC CRATE HEX SCALER REAL TIME CLOCK STEPPING MOTOR CONTROLLERS UP-DOWN COUNTERS V-F CONVERTERS (3) ION CHAMBERS (2) PREAMPLIFIERS (2) DIGITAL TO ANALOG CONVERTER
HUTCH DIMENSIONS:	SEE DIAGRAM ON FOLLOWING PAGE
STATUS:	OPERATIONAL
RESEARCH:	HIGH ENERGY EXAFS, GENERAL PURPOSE X-RAY, TOPOGRAPHY

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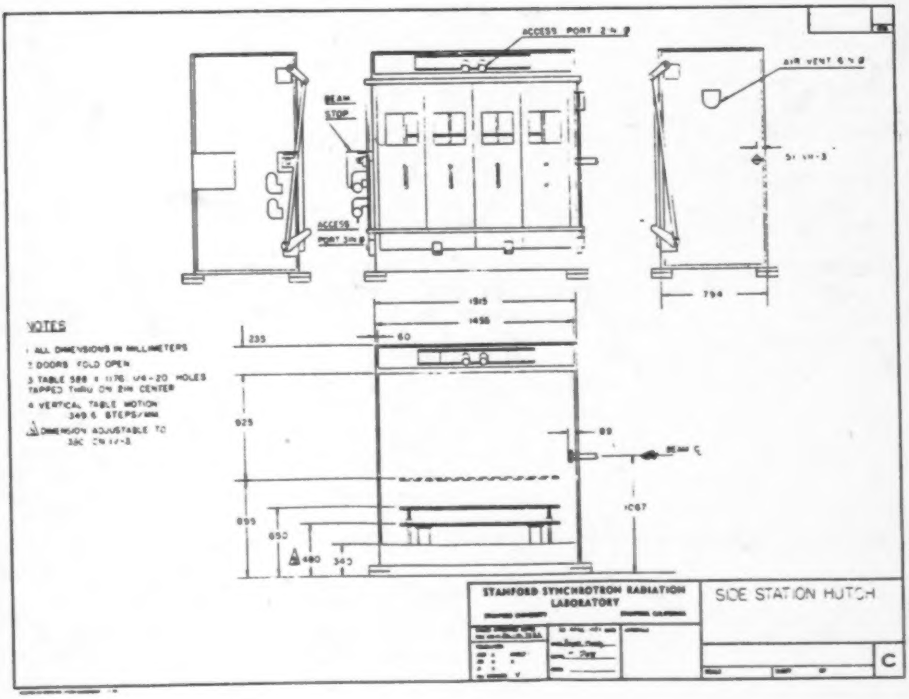
DIAGRAM OF A WIGGLER SIDE STATION
(Experimental Stations IV-1, IV-3 & VII-3)


ACCESS PORT 2¼ Ø
BEAM STOP
ACCESS PORT 3¼ Ø
AIR VENT 6¼ Ø
5¼ VII-3
794
1915
1498
235
60
925
89
BEAM ℄
1067
895
650
480
340
NOTES
1 ALL DIMENSIONS IN MILLIMETERS
2 DOORS FOLD OPEN
3 TABLE 588 × 1176 1/4-20 HOLES TAPPED THRU ON 2IN CENTER
4 VERTICAL TABLE MOTION 349.6 STEPS/MM
5 DIMENSION ADJUSTABLE TO 380 ON IV-3
STANFORD SYNCHROTRON RADIATION LABORATORY
SIDE STATION HUTCH
C

February 17, 1984

EXPERIMENTAL STATION 0-0 (90° UV-VIS, Lifetimes Port)

MIRROR:	POLISHED Be INSIDE SPEAR VACUUM SYSTEM DEFLECTS RADIATION RADICALLY OUTWARD (i.e. ANGLE OF INCIDENCE ON MIRROR IS 45°)
ENERGY RANGE:	APPROXIMATELY 1 eV - 6 eV DETERMINED BY "DYNASIL 1000" (Synthetic fused silica) WINDOW ON SPEAR VACUUM SYSTEM
ANGULAR ACCEPTANCE:	1.8 MRAD HORIZONTAL x 10 MRAD VERTICAL
ABSORPTION:	IN ADDITION TO WINDOW MENTIONED ABOVE THERE IS ABOUT 5 M OF FLIGHT-PATH VERTICALLY THROUGH AIR
SOURCE SIZE:	ELECTRON BEAM DIMENSIONS ARE ABOUT 4 mm HORIZONTAL x .4 mm VERTICAL LIGHT BEAM IN THE EXPERIMENTAL STATION IS ABOUT 4 cm HORIZONTAL x 1 cm VERTICAL
INSTRUMENTATION:	ORTEC PHOTON-COUNTING ELECTRONICS SPEX DOUBLEMATE MONOCHROMATOR WITH VARIOUS GRATINGS TRACOR-NORTHERN 1750 MULTI-CHANNEL ANALYZER AND DUAL FLOPPY DISC DRIVE HAMAMATSU R1333 PMT WITH COOLED BASE SOME OPTICAL COMPONENTS AND FILTERS
RESEARCH:	FLUORESCENCE LIFETIMES
REMARKS:	THIS PORT SHARES LIGHT WITH OPTICAL BEAM MONITORS USED BY SPEAR 90% FRONT-SURFACE Al BEAM SPLITTER IS INSERTED TO DIRECT LIGHT TO EXPERIMENTAL STATION. THE PULSE WIDTH IS 0.2-0.4 NSEC (measured: 550-700 psec) AND THE REPETITION RATE IS 1.28 MHZ IN THE SINGLE BUNCH MODE. EXPERIMENTS ARE PERFORMED IN A SHED ON TOP OF SPEAR SHIELDING.

SPECIALIZED INSTRUMENTATION

Specialized instrumentation available to users of SSRL includes an undulator, three diffractometers (Huber 6-circle, CAD-4 and a materials diffractometer), a VG Sample Chamber, a rotation camera, area detector for protein crystallograph a scattering camera. Because of the complexity of all of these instruments special training is required before they can be profitably used for research. In most cases, new user groups will be asked to send members in advance to serve an "apprenticeship" program with an experienced experimental group. The length of this training varies depending upon the new groups' familiarity with both diffractometers and SSRL monochromators. Approximate times are two weeks for persons unfamiliar with both, one week for persons already experienced with SSRL monochromator systems. Limited staff support is available for training on these instruments.

UNDULATOR

(Experimental Station IV-2 or VII-2)

A permanent magnet undulator is available as a high-brightness, quasi-monochromatic, tunable soft x-ray source. With SPEAR operating at 3.0 GeV, the fundamental peak can be varied from 750-1400 eV. With 100 mA stored current the on-axis brightness exceeds 10^{16} photons/sec mrad^2 within a 1% bandwidth.

Use of the undulator is limited due to the fact that it shares a beam line with a wiggler magnet. Utilization of the undulator requires removal of the wiggler magnet and also removal of the beryllium windows and x-ray monochromator. At present no soft x-ray monochromator is available for use with the undulator. However, the width of the fundamental peak is about 10% and this can be used directly.

For more information consult H. Winick or G. Brown.

March 22, 1984

HUBER DIFFRACTOMETER
(Experimental Station VII-2)

A Huber six-circle diffractometer is permanently installed on Beam Line VII-2 for high-resolution x-ray scattering research.

The six spectrometer degrees of freedom are (θ, ϕ) for the sample, and $(2\theta, \theta_c, \theta_d)$ for the detector. In addition, the input wavelength can be scanned, and the spectrometer coordinates can be remotely adjusted. Software is available for scanning between an arbitrary pair of reciprocal lattice vectors.

Because of very high demand, research is confined to problems that can only be addressed with this unique facility. Typical programs involve intrinsically weakly scattering systems, such as two-dimensional arrays and high resolution 3-D problems.

Users interested in use of the facility should contact George Brown.

THE CAD-4 SYSTEM
(Experimental Station II-2 or I-5)

BRIEF DESCRIPTION: The CAD-4 system consists of a single-crystal x-ray diffractometer which has been installed inside an SSRL radiation safety hutch and configured for multiple wavelength studies using synchrotron radiation. The system is mounted on wheels and can be used on any suitable x-ray station, however, it is generally stationed on I-5. It is ideally suited for multi-wavelength and/or polarization studies with small unit cell crystals.

INSTRUMENTATION: The CAD-4 system instrumentation consists of 3 major subsystems:

1. **Enraf Nonius CAD-4 Diffractometer:** A 4-Circle, Kappa geometry goniometer with factory standard components. The goniometer is mounted on its side with the theta axis in the horizontal plane (to take advantage of the horizontally polarized synchrotron x-rays).

2. **Incident X-Ray Beam Monitor:** At present this consists of an ionization chamber mounted ahead of the input beam collimator with associated current-sensing electronics to measure the incident beam flux. This measurement is necessary for proper scaling of the individual diffraction intensities when in the presence of a slowly varying input flux (typical for synchrotron radiation).

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3. **Remote Control Incident Beam Alignment Apparatus:** Four remote-controlled motions are provided to adjust the diffractometer relative to the incident beam: UP, DOWN, TILT, and SPIN. These adjustments are necessary for rapid realignment of the apparatus after installation on the x-ray station.

COMPUTER INTERFACE: At present the CAD-4 is controlled by coupled DEC PDP-8 and PDP-11 computers which are running the standard Enraf Nonius CAD-4 software (with a few minor changes). The PDP-8 controls the basic goniometer motions while the PDP-11 interfaces to the disc and tape drives (dual RK05's and TS03). The PDP-11 also interfaces to a camac crate for ancillary control and measurement operations (via a Borer type 1533 camac crate controller).

PHYSICAL CONSTRAINTS AND/OR LIMITATIONS: The diffractometer is mounted inside a radiation safety hutch which prohibits access during x-ray exposure of the crystal. Any experiments requiring manipulation of the crystal during exposure must be done using remotely actuated mechanical or electrical manipulators.

RESEARCH USAGE: The CAD-4 system is ideally suited for multi-wavelength and/or polarization studies with small unit cell crystals. Some examples of research in these areas which were performed using the CAD-4 system are:

1. Phillips, J.C., Wlodawer, A., Goodfellow, J.M., Watenpaugh, K.D., Sieker, L.C., Jensen, L.H., Hodgson, K.O. **Acta Cryst.**, A33, 445 (1976).
2. Phillips, J.C., Cerino, J.C., Hodgson, K.O. J. **Applied Cryst.** 12, 592-600 (1979).
3. Templeton, D.H., Templeton, L.K. **Acta Cryst.**, A36, 237-241 (1980).
4. Templeton, D.H., Templeton, L.K., Phillips, J.C., Hodgson, K.O. **Acta Cryst.**, A36, 436-442 (1980).
5. Templeton, D.H., Templeton, L.K., Phiackerley, R.P **J. Am. Chem. Soc.** 102, 1185-1186 (1980).

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SSRL MATERIALS DIFFRACTOMETER
(Experimental Station IV-3)

BRIEF DESCRIPTION: The SSRL Materials Diffractometer is a moderate size unit consisting of concentrically mounted Huber 421 (2θ axis) and 410 (ω axis) goniometers with z motion along the ω axis provided. These goniometers are stepper motor driven with choices of 200 or 2000 steps per degree. Optical rails have been mounted on both the instrument frame and 2θ arm and facilitate rapid setup of both input and exit slits and beam paths. A typical setup consists of input slits, I_0 detector, input beam path, sample cell, antiscatter slits, output beam path, exit slits, and I_1 detector. Data is collected as the ratio of I_1/I_0 to eliminate fluctuations in the input intensity.

DETECTORS: Various detectors are available, including in-line ion chambers, scintillators on photomultiplier tubes, and an energy dispersive Ge detector.

ALIGNMENT: The instrument has been constructed to simplify remote alignment. Vertical height and rotations of the entire instrument about χ and ω axes are stepper motor driven. Various accessories are available to simplify this process.

SAMPLE SIZE: Due to the side station installation, only relatively small samples or sample chambers can be accommodated. Approximate volumes must be contained in a cylindrical space about 20 cm diameter by 15 high, weight less than about 2 kg. The distance between sample and hutch wall is about 5 cm.

CONTROL SOFTWARE: Software is available to generate arbitrary motions in 2θ, ω, and incoming energy. Data collection scans can be taken with 2θ, or ω as the principal variable (standard diffractometer or rocking curve measurements) or with $k=4 \sin \theta/\lambda$ as the principal variable. These latter are particularly useful for comparing data taken at a variety of energies.

TYPICAL RESEARCH: Research to date has included anomalous scattering measurments to determine structures of amorphous materials and liquids, work on intercalated graphite and studies of large d-spacing Synthetic Layered Microstructures.

STAFF SUPPORT: Staff consultation is available in planning for experiments and a set of drawings of the instrument can be provided. A staff person will be available for consultation during initial instrument setup and alignment (approximately 1 shift) and "on call" thereafter to assist with instrument malfunctions. In view of the training program described in the introduction to this section, however, users will be expected to be essentially self sufficient otherwise. For further information, contact Denny Lorentz at Stanford University, (415)-497-1523.

February 17, 1984

VG SAMPLE CHAMBER
(Can be used on any VUV Experimental Station)

This system consists of a Vacuum Generators (VG) ADES 400 angular resolved photoelectron spectrometer and associated control units (this system does not have a cylindrical mirror analyzer but there is a port where one can be inserted). The pumping is done by a 400 ℓ/sec ion pump and a titanium sublimation pump. Two sample manipulators (also VG) are available for this system, however, users are advised to supply their own sample holders. The SSRL staff (Piero Pianetta) should be contacted for more details. Sample preparation capabilities include a sputter ion gun, variable leak valves and LEED optics. This sample chamber can be used on all the VUV lines without modification.

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SCATTERING CAMERA
(Experimental Stations I-5; II-2,3; IV-2,3; VII-3)

The SSRL Biotechnology program has supported the development of an x-ray scattering camera which can be used on a number of x-ray beamlines at SSRL. It consists of:

1) A collimation arm with two sets of Huber adjustable tantalum slits and an ionization chamber to measure the incident intensity.
2) A sample holder that is temperature regulated by a circulating fluid flow.
3) An evacuated scattering path with mylar entrance and exit windows and extension tubes allowing sample to detector distances of 20 cm through 70 cm (and up to 170 cm on II-2 with the hutch extension).
4) An intensity monitor (fluorescent screen/photodiode) in the tantalum beam stop.
5) A linear position-sensitive proportional counter of about 200 micron resolution and 6.38 cm useful active length.

Software exists for acquiring scattering data at a number of x-ray energies and storing the accumulated data on the beam line computer's disk memory. The Beam Line II-3 computer cannot run this program.

Experiments using this system to date have included large- and small-angle scattering studies of proteins in solution, large- and small-angle diffraction from proteins in oriented membrane pellets and concentrated non-crystalline protein samples and large-angle scattering from polymers. Interested users should contact Steve Hubbard (497-2479).

February 17, 1984

Area Detector for Protein Crystallography

The "Area Detector" facility for crystallographic data collection from macromolecules consists of a 2-dimensional multiwire proportional chamber mounted on a 5-circle Huber diffractometer. The energy of the x-ray beam is tuned by a 2-crystal monochromator and a platinum-coated mirror is used to eliminate the higher energy harmonics in the beam. Two ion chambers are used to measure the intensity of the incident x-ray beam and to measure x-ray absorption edges for wavelength calibration.

The facility is permanently in place at the end of the unfocused bending magnet Beam Line I-5, but access to the beam line is shared between the area detector station and the EXAFS I station which is located upstream on the same beam line. The facility was designed and developed to take advantage of the tunability of the synchrotron x-ray source and is used to measure crystallographic data at multiple x-ray energies selected to enhance anomalous scattering effects in the sample crystal with the intent of deriving x-ray phase information directly from the measured amplitudes.

The active surface of the area detector is approximately 25 cm x 28 cm, with a spatial resolution of approximately 2 mm. The crystal to detector distance may be varied from 30 cm to 100 cm, yielding sufficient angular resolution for use with sample crystals with unit cell edges of up to roughly 200 A. There is a temperature control system available which is nominally capable of maintaining the temperature at the sample to within 0.1°C. A locally developed program package supports sample crystal alignment, calibration of x-ray energy, crystallographic data collection, and processing of collected frame images to a list of partially corrected diffraction intensities.

This facility is primarily intended to measure enhanced anomalous scattering data for phase determination and although the overall system works well, it should be pointed out that this system is complex and the methodology and processing software are still being refined. Users interested in this facility should contact Paul Phizackerley on Ext. 2874.

February 17, 1984

Dedicated Rotation Camera Facility for Protein Crystallography (Branch Line VII-1)

An Enraf Nonius Rotation Camera for the photographic collection of crystallographic data from macromolecules has been installed on the 8-pole wiggler branch line VII-1. The high intensity beam available from the wiggler is focused by x-ray optical elements in both the horizontal and the vertical planes. This doubly-focused beam will facilitate the collection of data from (1) crystals with very large unit cells, (2) crystals with very small dimensions and (3) crystals which are radiation sensitive, since the effects of radiation damage normally do not take place immediately. It will also be possible to collect data more rapidly and to a higher resolution than with conventional sources. Since the energy of the beam is tunable, anomalous scattering data can be collected at elemental absorption edges.

This experimental station has been equipped with an enclosure for radiation protection that is the size of a small room. The enclosure incorporates an interlocked system of swinging bars that will provide easy access to the experimental apparatus without requiring intervention by an SSRL operator.

A cylindrically bent triangular crystal monochromator is used to focus 1.3 milli-radians of radiation in the horizontal plane. This crystal has an asymmetric cut which increases the intensity of the x-ray beam and also reduces the distance between the monochromator crystal and the focusing point at minimum x-ray bandwidth (the "Guinier" position). The monochromator is followed by a 58 cm. platinum-coated fused-silica x-ray quality mirror which is inclined to the incident x-ray beam to reject the higher energy harmonic components in the beam. The mirror can be bent to focus the beam in the vertical plane. A remotely controlled high-resolution TV camera, with a zoom lens, has been mounted inside the enclosure to simplify beam focusing and camera alignment.

The rotation camera, together with a set of tantalum X-Y slits, an ion chamber, a backstop and a film carousel, have been mounted on a 1 meter long optical bench, which is in turn mounted on an alignment carriage. This carriage is mounted on a second optical bench. These optical benches permit the focal distance and distances between individual components to be easily changed. The second optical bench is pivoted below the monochromator crystal and can be rotated about a vertical axis so that the x-ray wavelength can be readily changed over a large range. This will provide an opportunity to collect anomalous scattering data at any one of a large number of elemental absorption edges. However, it is expected that the system will normally be set to a given x-ray wavelength (such as 1.5418 Angstroms or 1.08 Angstroms) for extended periods of time and will be used primarily for the rapid collection of high quality diffraction data to high resolution and for the investigation of smaller and also radiation sensitive crystals.

February 17, 1984

The motions of all the optical elements and the rotation camera crystal phi axis and film carousel are under the control of a PDP 11/23 computer system through a CAMAC interface. Control software has been written for system alignment and data collection that is both flexible and straightforward to use. Furthermore, it will provide the capability of rotating the crystal phi axis at a speed determined by the incident x-ray flux, a normalization which makes the intensity of the recorded diffraction pattern independent of beam intensity fluctuations.

Sixteen flat film cassettes and four high resolution angled cassettes are available for data collection at this time. An FTS systems crystal cooling device that will provide temperature control at the sample position over the range -85°C to +100°C is also available.

An Enraf-Nonius x-ray generator, with a sealed fine-focus Cu tube has been fitted with a special collimator so that fiducial marks can be recorded on the x-ray film packs after exposure. There is also a precession camera (on the second x-ray port) for pre-alignment and screening of crystals, if desired.

A large darkroom has been constructed close to the camera. Temperature controlled processing tanks, complete with N_2 burst capability, have been installed. There are several wash tanks and three film driers. Ample bench and shelf space has also been provided together with a light box and a Supper circular film measuring instrument. SSRL will purchase x-ray film just prior to an experimental running period and keep the film refrigerated. The user would then be charged for the amount used. This will assure that fresh film is always available and will hopefully reduce the cost.

Crystal mounting equipment already exists in the biotechnology laboratory at SSRL and includes a stereo microscope, a Supper optical analyzer, assorted glassware and adequate bench space.

Currently we have no plans to provide a film densitometering and processing facility at SSRL. This decision is based on the fact that there are a large number of regional facilities already in existence throughout this country and furthermore that there are not sufficient staff members here to adequately support such a facility.

Scheduling.

Since branch line VII-1 will be used exclusively by the rotation camera facility, access to the facility will be permitted on a first come - first served basis. Please contact Ms. Carol Mitchell on Ext. 2874 for a Rotation Camera Beam Time Request Form. Users interested in further technical information should contact Paul Phizackerley at the same telephone number.

Prop. No._________

SSRL PROPOSAL SUBMITTAL FORM

This Proposal is a new proposal ( )
or a Replacement for Proposal No._____.

This Proposal is for a single experiment ( ) or a PROGRAM ( ).

CHECK MOST APPROPRIATE REVIEW PANEL:
X-ray Materials & Chemistry_____ VUV____ X-ray/Biology_____

---

1. TITLE: (10 words or less, type in capitals)

---

2. LIST OF COLLABORATORS (Underline Spokesperson)

Name	Full Address	Telephone Numbers Office	Telephone Numbers Home

3. EXPERIMENTAL STATIONS REQUIRED (If 2 stations required list both under first choice. Note number of shifts required on each station in section 4.)

First Choice: Alternates:

4. ESTIMATED DEDICATED BEAM TIME REQUIRED IN 8 HOUR SHIFTS:
(3 GeV,50 mA)

5. WILL IT BE POSSIBLE TO SCHEDULE SOME OR ALL OF THE EXPERIMENT IN PARASITIC TIME? IF SO, WHAT WOULD BE THE MINIMUM BEAM ENERGY?

6. For Experiments on Vacuum Beam Lines: List all samples you expect to insert into the vacuum system (and also lead time needed for preparation) and any construction materials and components not generally considered to be UHV materials or components. Details must be given in proposal.

7. LIST ALL POTENTIAL HAZARDS including all toxic, radioactive, or explosive materials, hazardous procedures and equipment. Furnish detailed safety procedures in the proposal. AGREEMENT TO BRING THESE MATERIALS TO SSRL MUST BE OBTAINED FROM J. CERINO, OPERATIONS MANAGER, AT LEAST 2 WEEKS PRIOR TO THEIR ARRIVAL.

8. What equipment or materials do you expect to be provided by SSRL?

9. PLEASE GIVE A BRIEF ABSTRACT OF THE PROPOSAL:

Prop. No.__________

SSRL PROPOSAL SUBMITTAL FORM

This Proposal is a new proposal ( )
or a Replacement for Proposal No._____.

This Proposal is for a single experiment ( ) or a PROGRAM ( ).

CHECK MOST APPROPRIATE REVIEW PANEL:
X-ray Materials & Chemistry_____ VUV____ X-ray/Biology_____

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First Choice:	Alternates:

4. ESTIMATED DEDICATED BEAM TIME REQUIRED IN 8 HOUR SHIFTS: (3 GeV,50 mA)

5. WILL IT BE POSSIBLE TO SCHEDULE SOME OR ALL OF THE EXPERIMENT IN PARASITIC TIME? IF SO, WHAT WOULD BE THE MINIMUM BEAM ENERGY?

6. For Experiments on Vacuum Beam Lines: List all samples you expect to insert into the vacuum system (and also lead time needed for preparation) and any construction materials and components not generally considered to be UHV materials or components. Details must be given in proposal.

STANFORD UNIVERSITY - STANFORD SYNCHROTRON RADIATION LABORATORY
User Agreement Application

Name of Applicant: ______________________ Telephone No ___________

Institutional Address: ______________________

____

Proposal Number(s): ______________________

(Check box as applicable in each classification listed below)

APPLICATION CLASSIFICATION - Applicant is a nonprofit organization or small business firm under Public Law 96-517, December 12, 1980. ____Yes ____No

USER CLASSIFICATION

☐ (1) SSRL facilities will be used in the performance of work under the Federal Government contract or grant identified hereunder:

Federal Agency ______________________

Grant # ______________________

Contract # ______________________

Principal Investigator ______________________

Title ______________________

Start Date ___________ Completion Date ___________

Patents Rights Clause (Reference) ______________________

(Copy must be attached)

Rights in Data and Copyright Clause (Reference) ______________________

(Copy must be attached)

☐ (2) SSRL facilities will be used in the performance of work by employees of the Federal Government.

☐ (3) Applicant is a foreign institution and SSRL facilities will be used in the performance of work fully supported by applicant, subject to the provisions of the international agreement between ______________ (country) and the United States of America identified below.

Title: ______________________

____

Dates (effective) ______________________

Applicable Clause (attach copy) ______________________

☐ (4) SSRL facilities will be used in the performance of work not subject to a Federal Government contract, grant or other pertinent agreement. Work performed by applicant will be at applicant's expense.

☐ (5) SSRL facilities will be used in the performance of work for User and not subject to a Federal Government contract, grant or other relevant agreement. SSRL will be reimbursed to the extent of full cost recovery.

TECHNICAL DATA CLASSIFICATION

The known requirements for technical data and the work to be performed as set forth in the proposals(s) are such that one of the following can reasonably be asserted:

____(1) There will be no technical data identification or restricted as being proprietary data.

____(2) The technical data identified in the attached list will likely be used in connection with the performance of the work and is represented as proprietary technical data subject to restricted access.

Applicant submits the proposals for performing experiments at SSRL identified above and represents that the classifications and statements as checked are correct.

Signature ______________________ Date ______________________

August 1983

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer:

- Development of surface-induced desorption EXAFS as a means of studying oxidation, corrosion and catalyst poisoning.
- Successful implementation of non-invasive angiography on dogs. This makes it highly likely that procedure will be applicable to humans opening up of 800-4000 eV range with the JUMBO monochromator. This made possible a variety of experiments on light elements
- First test of scanning soft x-ray microscopy.
- Development of photoelectron diffraction as a surface structural technique.
- Time-resolved small angle scattering used to study early stages of spinodal decomposition in a glass cooled from the melt, and polymer deformation kinetics.
- Development of x-ray undulator.
- Studies of phase transitions in two dimensions. New insights into range of correlations near the solidification temperature as a result of the high brightness from a wiggler.
- Development of grazing incidence diffraction studies of surface layers and extension of the technique to amorphous layers.
- Many studies of atomic coordinations and rearrangements in metalloproteins and metalloenzymes.
- Studies of chemical bonding of molecules and fragmentation processes on surfaces.
- Angle resolved Auger spectroscopy of chemisorbed systems.
- Characterization of interfacial structures on an atomic scale.
- Partial photoionization cross section determinations for the soft x-ray region.
- Angle resolved photoemission extended fine structure.

Research Highlights Anticipated for the Remainder of FY 1984 and FY 1985

SSRL is presently commissioning a 54-pole wiggler beam line which will increase our brightnesses and flux in the x-ray region by approximately 1 order of magnitude. This will make possible high resolution studies of two dimensional phase transitions, more definitive studies of amorphous thin films using grazing incidence diffraction and significant advances in time-resolved x-ray diffraction and absorption studies.

Similarly, we expect to implement a soft x-ray undulator beam line during the fall of 1984 and winter/spring of 1985. All the soft x-ray experiments at this Laboratory are presently photon flux limited. This new beam line should allow many significant advances there.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

   Answer: Major additions to the facility since October 1980 include: development of the first double-crystal monochromator in the soft x-ray region; the development of focusing optics for a wiggler beam line; completion of a second wiggler beam line and an accompanying 6-circle diffractometer for scattering studies; three additional stations on the two wiggler beam lines; a station for lithography-microscopy; the development and implementation of an area detector; development of the first 54-pole wiggler beam line; development of the first soft x-ray undulator insertion device; and the first wiggler station dedicated to protein crystallography.

   Plans for the next year and a half include the development of a beam line with three experimental stations for VUV research based on three interchangeable undulator insertion devices; the construction of a fourth wiggler and a fourth bending magnet beam line; an array of improvements to the storage ring SPEAR, which will enhance its operation as a synchrotron radiation source; an undulator beam line on the storage ring PEP, which will provide the most intense source of x-rays available for the next decade; and the provision of an injection device, which will allow SPEAR to operate for synchrotron radiation during times when this is presently not possible.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

   Answer:

(Budget Authority in Thousands)

	81*	82*	83	84	85
A. BES OE & CE Funding					
Nuclear Sciences			6344	6736	7980
Materials Sciences			0	700	1700
			6344	7436	9680
CE Funding					
Nuclear Sciences			456	490	600
Materials Sciences			0	100	300
Total CE			456	590	900
Total OE&CE			6800	8026	10580
B. OE & CE Distribution					
Operating OE			6192	6577	7980
Operating CE			31	57	285
Total Operating			6223	6634	9070
In-House Research OE			152	859	895
In-House Research CE			425	533	615
Total Research			577	1392	1510

(Budget Authority in Thousands)

	81*	82*	83	84	85
C. Other Funding					
GPP			0	0	100
AIP			0	0	0
SSRL Enhancement PE&D			100	350	0
SSRL Enhancement Construction			0	940	9130
Energy Management			0	0	0
			100	2790	10230
D. Out-of-House Research			0	0	0

*NSF funded

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer:

(Budget Authority in Thousands)

	81*	82*	83	84	85
OPERATIONS					
OTHER FEDERAL SOURCES	5455	5394	635	467	467
OTHER NON-FEDERAL SOURCES	117	134	198	138	150
	5572	5528	833	605	617
CONSTRUCTION					
OTHER FEDERAL SOURCES	0	770	902	803	0
OTHER NON-FEDERAL SOURCES	209	1430	916	475	0
	209	2200	1818	1273	0

*NSF provided the principal support for SSRL until FY 1983, when it was transferred to DOE.

8. **For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.**

Answer:

DOE SUPPORTED SSRL STAFF - FY'81 - FY'85
NUMBER OF INDIVIDUALS

	PERMANENT STAFF	GRADUATE STUDENTS	OTHER**	TOTAL
FY'81*	49	5	1	55
FY'82*	50	7	6	63
FY'83	54	7	10	71
FY'84	57	10	6	73
FY'85	68	12	7	87

*NSF Supported in '81 & '82

	PERMANENT STAFF	GRADUATE STUDENTS	OTHER**	TOTAL
Other Supported SSRL Staff - FY'81 - FY'85				
FY'81	3	1	0	4
FY'82	6	2	0	8
FY'83	10	5	0	15
FY'84	10	5	1	16
FY'85	10	6	2	18

**Other includes temporaries and visiting scientists on payroll.

9. **What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?**

Answer: SSRL is always fully utilized since the facility is oversubscribed by approximately 50%. The definition of full utilization is 24 hour, 7 day per week use of each experimental station (either for data taking, set up for data taking or facility development) at times in which photons usable by the station are delivered from SPEAR. (Note: The SLAC linac is shut down approximately 4 months a year. The remaining 8 months are shared 50% between production dedicated to synchrotron radiation, and a SLAC high energy physics program. During the dedicated portion, all 18 SSRL experimental stations are fully utilized. During the high energy colliding beam portion, 11 of the experimental stations are utilized.)

10. **For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?**

Answer: We expect approximately 450 proposals to have been submitted in this time period, similar to the number submitted in the period of January 1979 to January 1984. There is a growing number of program proposals, which use more time at SSRL, rather than single experiment proposals. Of the 450 approximately 320 will have been started, 260 of these 320 will be continued and 160 completed (some of them having been started before FY 1981).

11. **What is this facility's user policy?**

Answer: SSRL is open to all users on the basis of scientific competition. There are no charges for the use of the experimental facilities, except for proprietary research. This policy was put in place in 1975 by agreement with the National Science Foundation, the agency then supporting operation of SSRL. The policy has been very productive of excellent scientific results and has contributed strongly to the United States' position of leadership in synchrotron radiation research.

12. **For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?**

Answer: The only research performed at SSRL which is reimbursable is proprietary. In the period FY 1981 to present, no reimbursable research was performed. It is anticipated that proprietary research will be done at the facility in the remainder of 1984 and in 1985. Revenues from this reimbursable research are estimated to be $3,000 in 1984 and $5,000 in 1985.

13. **What is the mechanism by which specific research proposals for experiments at the facility are considered?**

Answer: Proposals are ranked on the basis of scientific merit by an outside panel of 10 scientists. Prior to this ranking, a peer review process occurs during which 2-6 reviews are obtained on each proposal. Experimental time is assigned at SSRL based on the ratings of the panel.

14. **How many research proposals have been submitted over the past five years, and how many of these have been approved?**

Answer: Four hundred forty-four proposals have been submitted since January 1979. Proposals to SSRL are not accepted or rejected but ranked on the basis of scientific merit. Approximately 10% of the proposals receive ratings too low to be considered for experimental time.

15. **How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?**

Answer: Approximately 370 university personnel have utilized the facility in the past 5 years.

16. **How many industrial researchers have utilized the facility over the past five years?**

Answer: Approximately 135 industrial researchers have worked at SSRL in the past 5 years.

17. **How many researchers from foreign institutions have utilized the facility over the past five years?**

Answer: Approximately 75 researchers from foreign institutions have utilized SSRL in the past five years.

18. **How many researchers from other agencies have utilized the facility over the past five years?**

Answer: Approximately 115 scientists from other DOE-funded laboratories have utilized SSRL in the last five years. Approximately 30 scientists from other Government Laboratories have used SSRL.

19. **What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?**

Answer: Included in the FY 1985 appropriation is funding for an enhanced beam line at the SSRL which would be the first hard x-ray undulator beam line in the world and in addition, funds have been appropriated to house the experimental station. Also included in the appropriation is funding to reduce the emittance of the SPEAR ring, to add an injector which would be usable at times when other sections of the SLAC LINAC are not functioning and to reduce the beam vibration on SPEAR.

20. **Please provide a copy of the facility's latest annual report.**

Answer: Attached. [Note: Excerpts from this report follow.]

SSRL

Arthur Bienenstock
Director

Herman Winick
Deputy Director

SSRL REPORT 84/01
Activity Report for
April 1, 1983 - December 31, 1983

Edited by Katherine Cantwell

ABOUT THE STANFORD SYNCHROTRON RADIATION LABORATORY

SSRL is a national facility supported primarily by the Department of Energy for the utilization of synchrotron radiation for basic and applied research in the natural sciences and engineering. It is a user-oriented facility which welcomes proposals for experiments from all qualified scientists.

The synchrotron radiation is produced by the 4 GeV storage ring, SPEAR, operated by the Stanford Linear Accelerator Center (SLAC). The storage ring is dedicated to the production of synchrotron radiation during 50% of its operations time or about 4 months per year. The remainder of the time synchrotron radiation may be used parasitically during colliding beam runs for high energy physics experiments.

SSRL currently has 18 experimental stations with 9 more proposed to be built within the next three to four years. There are 196 active proposals for experimental work from 102 institutions involving approximately 550 scientists. There is normally no charge for use of the facility by experimenters.

Additional information for prospective users is contained in the booklet "SSRL Proposal Guidelines and General Information". This booklet and further information about the facility may be obtained by writing or telephoning Katherine Cantwell at SSRL, SLAC Bin 69, P.O. Box 4349, Stanford, CA 94035 - telephone (415) 854-3300 ext. 3191.

This report summarizes the activity at SSRL for the period April 1, 1983 to December 31, 1983.

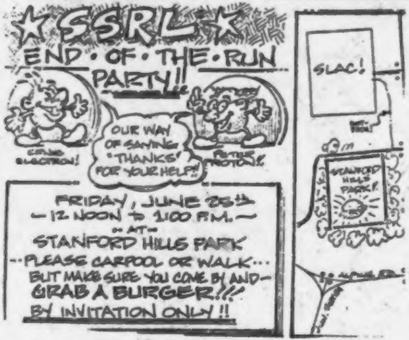
SSRL is supported by the Department of Energy, Office of Basic Energy Sciences; the National Science Foundation, Division of Materials Research; and the National Institutes of Health, Biotechnology Resource Program, Division of Research Resources.

Photograph by H. Morales and S. Brennan

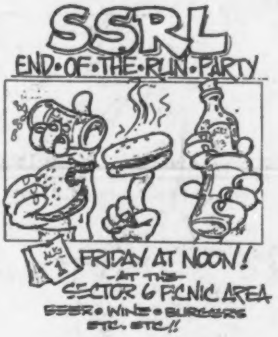
A very powerful beam of synchrotron radiation x-rays striking a silicon crystal. The beam is produced by a 54 pole permanent magnet wiggler operating in the SPEAR storage ring at SSRL. The x-rays are incident from the right with an intensity that is so high that a visible flourescence can be seen in the helium gas plus a particularly bright spot where it strikes the silicon crystal in the center of the photograph. The 54 pole wiggler and the associated beam line are a joint project of the EXXON Corporation, the Lawrence Berkeley Laboratory and SSRL.

THIS REPORT IS DEDICATED TO NORMAN SILVEIRA

Norman Silveira, Draftsman and Graphic Illustrator, contributed greatly to SSRL over the past four years. His drawings brought us pleasure. Norman died in an auto accident March 16, 1984. We will miss him.

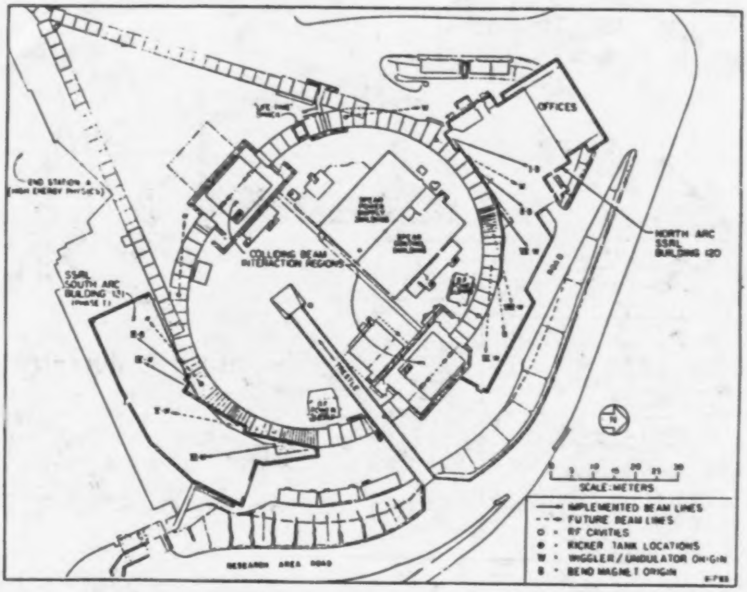

★SSRL★
END • OF • THE • RUN
PARTY!!
ELECTRON!
PROTON!
OUR WAY OF SAYING "THANKS" FOR YOUR HELP!!
FRIDAY, JUNE 25th
— 12 NOON TO 1:00 P.M. —
— AT —
STANFORD HILLS PARK
--PLEASE CARPOOL OR WALK...
BUT MAKE SURE YOU COME BY AND—
GRAB A BURGER!!!
BY INVITATION ONLY!!
SLAC!
STANFORD HILLS PARK!

Stanford University


SSRL
END • OF • THE • RUN • PARTY
AUG 1
FRIDAY AT NOON!
— AT THE —
SECTOR 6 PICNIC AREA
BEER • WINE • BURGERS
ETC. ETC.!!

STANFORD SYNCHROTRON RADIATION LABORATORY

SITE PLAN


END STATION A
(HIGH ENERGY PHYSICS)
OFFICES
COLLIDING BEAM
INTERACTION REGIONS
NORTH ARC
SSRL
BUILDING 120
SSRL
SOUTH ARC
BUILDING 121
(PHASE I)
ROAD
TRESTLE
RESEARCH AREA ROAD
N
0 5 10 15 20 25 30
SCALE: METERS
IMPLEMENTED BEAM LINES
FUTURE BEAM LINES
○ - RF CAVITIES
● - KICKER TANK LOCATIONS
W - WIGGLER/UNDULATOR ORIGIN
B - BEND MAGNET ORIGIN

SSRL is contained in two buildings adjacent to the storage ring SPEAR at the Stanford Linear Accelerator Center. The North Arc Building houses Beam Lines I, II, and VII and the South Arc Building Beam Lines III, IV and VI. The locations of future Beam Lines V, VII and IX are indicated.

I OVERVIEW

-Arthur Bienenstock-
Director

SSRL has entered its second decade. The major emphasis of the last 10 years has been on developing and exploiting the capabilites of SPEAR as a synchrotron radiation source and establishing a smoothly operating user experimental facility. In the next decade it is time to turn our attention to the development of the next generation of sources and technology based on insertion devices. Towards this end a strong machine physics group has been established at SSRL during the last six months.

At present there are six new beam lines and three new experimental stations in various states of planning, construction or commissioning. Beyond these near-term developments the Laboratory is looking towards the exploitation of the PEP storage ring as a synchrotron source as well as design and construction of a new 6 GeV storage ring dedicated to synchrotron radiation.

The most striking accomplishment of the past six months has been the completion of the SSRL/LBL/EXXON 54-pole wiggler line. This beam line will provide about a factor of five increase in photon flux and brillance for SSRL users.

The Stanford Enhanced Photon Flux Facility (SEPFF) has become a reality. This project will contribute to the Laboratory in a variety of ways. The most exciting of the these is the development of an undulator beam line on the storage ring PEP. This beam line will provide another order of magnitude increase in brillance over the 54 pole wiggler on SPEAR. In addition, it will pave the way for future beam lines on PEP.

A third PRT beam line was accepted by SSRL early this fall. This PRT is a collaboration between the University of California and the National Laboratories. This group plans to construct two beam lines, one from a wiggler and one from a bending magnet source. A toroidal grating monochromator will be placed on the bending magnet line opening the spectral gap between the present 8° line and the grasshoppers (25-75 eV) to exploitation. The wiggler line will contribute another source of hard x-rays to the user community. Presently, wiggler beam time is greatly oversubscribed.

In December, light was delivered to the new Protein Crystallography Rotation Camera located on a wiggler side station. This facility will open to Users in March, 1984.

A New Rings Workshop held in July generated much excitement about the scientific possibilities of a 6 GeV storage ring. Plans for such a ring are actively underway.

HIGHLIGHTS OF SCIENTIFIC RESULTS

The following is a brief synopsis of some of the highlights of research results at SSRL during the past six months. More information can be found in Section IX under the reports for the relevant proposals--as indicated by the numbers in parentheses.

In areas related to the biotechnology activities at SSRL there have been major advances in both instrumentation and use of SSRL for scientific and technological studies. The area detector facility for protein crystallography has been fully operative during the past year (651) and was used to collect high resolution anomalous scattering data on several proteins. A new rotation camera beam line is just being commissioned which will provide extremely high flux for the collection of protein diffraction data in a user friendly mode.

The utilization of small angle scattering for studying conformation and structure of biological molecules continues to increase and show promising results. Such studies include binding of ions to the acetylcholine receptor (707) and the conformational changes of regulatory proteins in solution (712). Recent results on surface scattering from phospholipid arrays show promise for leading to the determination of structural information by diffraction for these systems (748).

EXAFS and edge studies of metalloproteins continue to utilize a large amount of beam time and produce new scientific results. Among the highlights of the past year are studies resolving the controversy surrounding the nature of the three iron site in ferredoxins (762) and further studies of heme proteins such as cytochrome oxidase (632) and cytochrome P-450 (699). Significant progress is being made toward the development of techniques for doing time resolved EXAFS and edge studies of intermediates (663 and 659).

Synchrotron radiation at SSRL is continuing to play a role in medicine. EXAFS studies are being used to study the in vivo nature of gold anti-arthritic drugs (559). Angiography experiments continue to improve with successful imaging of dog hearts. Plans are now underway to widen the central beam on line IV-2 to provide a 12-15 cm beam by next fall. This will allow the first human trials of the angiography procedure.

Thirty-one progress reports were filed this year with subjects embracing the nonbiological applications of x-ray research in condensed matter physics. The techniques of EXAFS, small angle scattering, high-resolution scattering, and x-ray topography were applied to a wide variety of physical and chemical systems. In what follows, the highlights of the 19[illegible] research efforts will be briefly discussed.

High-resolution diffraction experiments on two-dimensional and quasi-two-dimensional systems continue to yield important new results. The phase diagrams of lead on copper (608), ethylene on graphite (720), krypton on graphite (813), are now known in far greater detail. The molting of xenon monolayers on a single cryctal of graphite has been studied for the first time (742), demonstrating the persistence of angular correlations a few degrees above the melting temperature. Much more detailed experimental work has been performed on the phase diagrams of freely suspended liquid crystals (716), as well as on freely suspended strands of discotic liquid crystals (792).

The structure of liquids and amorphous solids was the subject of several investigations. Amorphous Mo-Ge alloys (639), molten Se_xTe_{1-x} (788), Hg complexes in solution (700), amorphous Fe_xGe_{1-x} alloys (814), lunar glasses (615), BeF_2 glasses (434), $Ni_{66}Be_{33}$ glasses (683), and $GeBr_4$ glasses (706) were studied. Radial distribution functions have been obtained on amorphous thin films of $GeSe_2$ with and without Ag photodiffused into the material (789).

Investigations of structures of catalytic interest focused upon mixed-organometal clusters (777), and supported metal catalysts under conditions of CO chemisorption (471). Also of technological interest are the investigations of potassium in coal (647), and sulfur in coal (469). The latter studies made use of a carefully designed fluorescence spectrometer that permits conventional (nonvacuum) spectroscopy at energies as low as 2.4 keV (678).

Progress reports in the VUV/Soft X-ray area show that a continually active field has been studies of photoionization phenomena at the ionization threshold of core levels and in valence band levels, as well as the mapping of the energy dependence of partial photoionization cross sections above the threshold. Fragmentation of small molecules when passing through the excitation energies for the C 1s, N 1s and O 1s core levels has been examined by simultaneous defection of Auger decay electrons and ionic fragments (810). Resonance photoemission has been applied to narrow-band materials containing 4f and 5f electrons (682) and for rare-earth metals (771). Similarly resonant interchannel coupling and asymmetry parameters over a large photon energy region have been determined for simple gases (523, Part III-B). Effects of the solid state or the energy dependence of partial cross-section has been addressed for the first time in a systematic way (772).

High resolution core level spectroscopy has been applied to surface shifts for CO and NH_3 chemisorbed on Pt and for O_2 onto W (614).

Angle-resolved photoemission has been used to investigate the magnetic-electronic structure of Cr, an antiferro magnetic material (523, part IV-1). Polarization dependent near-edge structure absorption measurements on a single crystal of graphite have demonstrated that the symmerty of the final state can be determined (737).

Surface and interface studies regarding both electronic and structural terminations have continued to receive great attention. Chemical reactions at metal-semiconductor (Si, III-V's) interfaces (616,771) and microscopic models to understand Schottky barriers in III-V's have been studied extensively (616), as well as band-edge discontinuities in Ge/Ge/GaAs hetero structures (652) and surface electronic structure of GaAs (756). Both bulk and surface investigations have been made of a more complex semiconductor alloy, $Hg_{1-x}Cd_xTe$ (616).

The coordination chemistry of metal oxide and chloride surfaces has been studied with focus on assignment of the orbited symmetry of the valence band levels (733).

The reflectivity of synthetically fabricated multi-layer coatings for mirrors has been tested in the spectral region 80-1000 eV (776). The results are very encouraging with important implications for future developments of soft x-ray optics.

II REVIEW OF LABORATORY OPERATIONS

INTRODUCTION

The last six months have seen some of the best and some of the worst SPEAR running in recent years. Both the parasitic and dedicated runs in the spring of 1983 were extremely smooth. The May-June run was the longest (149 scheduled SPEAR shifts) to date.

Fall 1983 SPEAR operations started in early October in the parasitic mode. The luminosity for colliding beam running appeared to be down by a significant factor. After a month of virtually no usable beam for either SSRL or the high energy physics program, SSRL agreed to start dedicated operation two weeks earlier than originally scheduled. On November 7, the facility went dedicated on a week's notice. As of the end of December, the luminosity problem appears to be resolved and normal spring operation is anticipated.

Between October and Christmas, a third of the 202 scheduled shifts were used for Machine Physics aimed, primarily, at understanding the cause of the decreased luminosity. In addition, SSRL pursued several machine physics projects as described in Section III.

DEDICATED RUNNING

Since October 1979, SPEAR has operated 50% of the time in a mode dedicated to synchrotron radiation production. From January 1, 1983 to December 31, 1983, a total of 306 dedicated 8-hour SPEAR shifts were provided. These shifts, divided into three separate runs, resulted in a total of 3523 user shifts on the 16 SSRL experimental stations.

PARASITIC RUNNING

Since 1979, 66% of the colliding beam running has been at energies below 2.0 GeV. Much of this low energy running has been at 1.5 GeV. At this energy, the wigglers are not operated. At 1.8 GeV the critical energy from the bending magnets is only 1.0 keV, providing no useful photon flux to x-ray stations which generally operate above about 4-5 keV. On the wiggler lines the critical energy is 3.9 keV at full field so that usable intensity is produced at x-ray energies with the enhancement due to the 8 wiggler poles. In parasitic conditions stored current is limited by the beam-beam interaction to about 5 mA at 1.5 GeV and about 12 mA at 2.0 GeV. The beam emittance is enlarged by the counter-rotating positron beam resulting in a flux per mA that is reduced by a factor of 2-5 for most experiments compared to single beam, dedicated operation.

During this reporting period the bending magnet x-ray lines were closed during parasitic operation. However, the VUV lines, the lifetimes port and the five wiggler stations operated for certain types of experiments. 660 parasitic user shifts were employed for experimental work. Much facility development work also occurs during parasitic operation.

TIMING MODE OPERATION

In order to allow experimental groups to take advantage of the unique timing properties of SPEAR, approximately 20% of dedicated running is in the timing mode. Timing mode is four individual bunches of electrons equally spaced in the SPEAR ring and therefore separated by 190 ns. Standard dedicated operation is four equally spaced groups of four adjacent bunches. Adjacent bunches are 2.8 ns apart. Improvements in the SPEAR vacuum system were made over the summer which appear to have decreased the higher order heating mode problems which previously limited the current in timing mode. Currents equivalent to multi-bunch operation are now expected. However, the stored electron lifetimes are approximately 50% less than in multi-bunch operation. The bunch length is about 300 ps (FWHM), the minimum bunch spacing is 2.8 ns and the orbital period is 760 ns. Timing mode operations occurred from June 16-30 (39 shifts) during this reporting period.

BEAM AND SPEAR USAGE TABLES

The following Tables contain statistics on SPEAR running, experimental use and characteristics of SSRL stations. For earlier information consult previous Activity Reports.

Table II-1 shows the number of parasitic shifts by energy since 1979 when dedicated running commenced.

Table II-2 shows the performance of the SPEAR storage ring during dedicated running. The May-June 1983 dedicated run was very smooth with stable beam delivered 80% of the scheduled time. The fall 1983 run experienced an average 77% delivery of stable beam. However, the run had a very shaky start and an excellent finish. The average in November of only 70% delivery improved in December to 83%.

Tables II-3 and II-4 illustrate the use of beam at SSRL for experimental purposes. The number of users per dedicated shift averaged 11.5 for this year. The average number of shifts used during each assignment to a proposal under dedicated running was approximately 15, as it has been for a number of years.

Table II-5 represents the number of shifts requested versus the number of shifts actually assigned for the fall dedicated period. Last May's Activity Report contains similar figures for October 1982-June 1983. Demand continues to significantly exceed available time at the facility. During this period the three wiggler side stations experienced the highest demand. Over the last two years may experimenters have redesigned their equipment to accommodate these small hutches. Increased demand for the bending magnet x-ray lines reflects both the improvements to Beam Line II over the last year and the semi-dedication of

I-5 to the Area Detector. This Table shows that a significant number of proposals do not receive beam time in any given period. However, due to the collaborative nature of most proposals there are only a handful of individual scientists who have applied to the Facility who do not receive any beam time in a given year through various collaborations.

Table II-6 is a listing of the characteristics of the SSRL experimental stations.

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TABLE II-1

DISTRIBUTION OF PARASITIC SHIFTS BY STORED BEAM SINCE 10/79[*]

PERIOD	1.5-1.99 GeV	2.0-2.4 GeV	2.5 GeV	TOTAL
11/-12/79	6	57	0	63
02/-07/80	9	160	15	184
10/-12/80	114 (1.55 GeV)	0	0	114
03/-05/81	96	0	121[**] (3.7 GeV)	217
10/-11/81	87	41	0	128
02/-03/82	38	0	0	38
04/-06/82	139	0	0	139
11/-12/82	122	0	0	122
02/-05/83	125	0	0	125
10/-11/83	30	0	0	30
TOTALS	766 66%	258 22%	136 12%	1160 100%

[*] (Commencement of 50% dedicated operation)

[**] Beam instabilities and frequent unscheduled dumps resulted in poor conditions for SSRL experimenters during much of this run.

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TABLE II-2

Beam Time Statistics/DEDICATED TIME

STORED BEAM TIME					NON-STORED BEAM TIME				
					TOTAL		DISTRIBUTION		
PERIOD	Scheduled Hours	Stored Beam Hours	Number of Proposals Run	Energy GeV	Non-Stored Hours	Filling & Tuning	SPEAR Down	Linac Down	Access Time
10/20-11/5/79	152	95.3	10	2.6	56.7 (37%)	20%	45%	29%	6%
12/3-12/21/79	352	299.4 (40.7)*	31	3.0	52.6 (15%)	49%	21%	24%	6%
2/8-3/5/80	472	366.3 (13.3)	29	3.0	105.7(23%)	68%	9%	14%	9%
4/16-5/19/80	764	588.2	46	3.1	175.9(23%)	63%	25%	10%	2%
6/30-7/30/80	726	320.4 (22)	48	3.0	** 405.6(56%)	29%	34%	37%	0%
9/29-10/14/80	336	194.9	13	3.0	141.1(42%)	51%	10%	39%	0%
12/2-12/22/80	440	309 (25.5)	25	3.0	131 (30%)	72%	20%	8%	.01%
1/26-3/3/81	792	600.9 (16.1)	41	3.0	191.1(24%)	60%	10%	23%	6%
5/16-6/30/81	988	727 (26.7)	74	3.0	*** 261 (26%)	47%	23%	29%	1%
11/18-12/21/81	546	363.6 (52.9)	37	3.0-3.5	182.4(33%)	52%	18%	24%	6%
1/18-2/22/82	748	612.5 (33.9)	52	3.0	135.7(18%)	45%	22%	30%	3%
3/9-4/26/82	995	830.9 (66)	64	3.0-3.4	164.1(16%)	53%	33%	5%	8%
10/15-11/5/82	473	316	49	3.0-3.4	157 (23%)	43%	25%	30%	2%
12/27/-2/22/83	1050	825.6	73	3.0	224 (21%)	39%	45%	14%	1%
5/9/-6/30/83	1195	960.3	93	3.0-3.4	234.7(20%)	37%	26%	35%	2%
11/7-12/23/83	857	662.8	65	3.0	194.2(23%)	54%	17%	19%	10%

* At certain times (e.g., machine physics studies on the Linac) SPEAR injection is uncertain. These times are not considered scheduled beam time for SSRL experiments. However, some time is often available. The additional hours beyond the scheduled stored beam hours are indicated in ( ).

**Frequent power brown-outs occurred during this period.

***Beam instability & frequent unscheduled dumps resulted in poor conditions for SSRL experimenters during much of this run.

TABLE II-3

SHIFTS USED & PROPOSALS RUN

RUN PERIODS	12/27/82 to 02/22/83	02/23/83 to 05/09/83	05/09/83 to 06/30/83	10/17/83 to 11/07/83	11/07/83 to 12/23/83	TOTALS for PERIOD
User Shifts (Parasitic)	-	629		31		660
User Shifts (Dedicated)	1210		1349		964	3523
Proposals Run (Parasitic)		29		4		31
Proposals Run (Dedicated)	73		93		65	231
Users/Shift (Parasitic)		5.0		1.2		4.3
Users/Shift (Dedicated)	11.7		11.2		11.6	11.5

Axel Golde and Bob Filippi, long time members of the SSRL staff, relaxing at the Users Conference. Axel has been responsible for facility construction since the very beginning of SSRL and Bob for the fabrication of much of the experimental workings of SSRL (beam line components, instrumentation, and all manner of general nuts and bolts).

SUMMARY OF SHIFTS USED FOR SSRL EXPERIMENTS

Dates of Runs	1-1	1-2	1-4	1-5	2-2	2-3	2-4	3-1	3-3	3-4	4-1	4-2	4-3	7-2	7-3	0-0	User Shifts	SPEAR Shifts	Users/SPEAR Shifts
1/18-2/22/82 Dedicated	71	59	64	67	66	61	54	72	76			70	64	73	71	15	883	93	9.5
2/23-3/9/82 Parasitic	35	0	0	15	0	0	0	35	0			0	0	0	0	35	120	38	3.2
3/9-4/26/82 Dedicated	89	87	76	96	80	69	87	103	103	56		83	73	99	100	15	1216	112	10.9
4/26-6/15/82 Parasitic	44	35	0	0	0	0	0	75	0	32		0	0	0	0	0	186	120	1.5
10/15-11/5/82 Dedicated	40	30	34	29	32	30	40	27	22	0		31	36	37	37	0	425	40	10.6
11/5-12/22/82 Parasitic	54	48	0	0	0	0	9	51	39	0		51	38	26	34	53	403	100	4.0
12/27-2/22/83 Dedicated	98	111	72	91	86	78	63	101	93	38		83	94	85	99	18	1210	103	11.7
2/23-5/9/83 Parasitic	59	59	0	0	0	0	0	109	94	0		71	48	56	43	90	629	125	5.0
5/9-6/30/83 Dedicated	113	113	85	67	107	78	74	107	82	0	88	112	102	116	105	0	1349	120	11.2
10/17-11/7/83 Parasitic	0	0	0	0	0	0	0	0	9	0	3	4	4	6	0	9	35	30	1.2
11/7-12/23/83 Dedicated	69	71	41	75	65	46	37	65	51	0	75	79	76	83	80	51	964	83	11.6
TOTALS	672	613	372	440	436	362	364	745	569	126	166	584	535	581	569	286	7420	964	7.7

TABLE II-4

The figures on this chart do not include time used for set-up and testing of facility equipment or beam lines.

TABLE II-5

DEDICATED DEMAND vs ACCOMMODATION ON SSRL EXPERIMENTAL STATIONS

September 1983 - December 1983*

Experimental Station	Shifts Requested	Shifts Assigned	% Assign	Proposals Requested	Proposals Assigned*	% Assign
X-ray (Bending Magnet)	593	217	37%	35	16	46%
Wiggler (End Station)	340	130	38%	15	7	47%
Wiggler (Side Station)	653	146	22%	46	11	24%
Grasshoppers (VUV)	297	120	40%	9	4	44%
8° (VUV)	56	56	100%	2	2	100%
Jumbo (VUV)	130	57	44%	5	2	40%

*Figures based on originally anticipated dedicated schedule.

photo by H. Winick

Ann Waldheuer and Mike Rowen of the VUV staff working on the Jumbo Monochromator

(Branch Line III-3)

CHARACTERISTICS OF SSRL EXPERIMENTAL STATIONS

	Horizontal Angular Acceptance (Mrad)	Energy Range (eV)	Resolution	Approximate Spot Size Hgt x Wdth (mm)	Remarks
Beam Line I					
1-1 (4°)	2.0	32-1000	$\Delta\lambda=.1-.2$A	2.0 x 1.0	Double Focus
1-2 (8°)	4.0	4-40	$\Delta\lambda=.2-6$A	1.0 x 3.0	Highly Polarized Double Focus
1-4 (Curved Crystal)	2.2	6000-9500	~ 60 eV	0.25 x 0.5	Double Focus Scattering
1-5 (EXAFS I)	1.0	3800-29300	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Beam Line II					
II-2	4.8	2800-8900	$\Delta E/E \sim 5x10^{-4}$	2.0 x 4.0	Rapidly Tunable
II-3	1.0	2800-30000	$\Delta E/E \sim 5x10^{-4}$	2.0 x 20.0	Rapidly Tunable
II-4	1.0	3200-30000	White Radiation	4.0 x 15.0	
Beam Line III					
III-1 (4°)	2.0	15-1200	$\Delta\lambda=.05-2$A	1.0 x 1.0	Double Focus
III-2 (18°)*	8.0	4-150	$\Delta E/E \sim 10^{-3}$	1.6 x .25	Differentially Pumped
III-3 (2°)	8-10	800-4000	0.35-7 eV	2.0 x 4.0	Ultra High Vacuum
III-4 (3°)	2.0	2-3000	White or $\Delta\lambda/\lambda=.01$	2 x 8	Differentially Pumped
Beam Line IV (Wiggler)					
IV-2					
Unfocused	1.0	2800-45000	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Focused	4.6	2800-10200	$\Delta E/E \sim 5x10^{-4}$	2.0 x 6.0	
IV-3 & IV-1	1.0	2800-45000	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Beam Line VI (Wiggler)					
VI-2					
Unfocused	1.0	2800-45000	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Focused	3.0	2800-21000	$\Delta E/E \sim 5x10^{-4}$	2.0 x 6.0	
Beam Line VII (Wiggler)					
VII-2					
Unfocused	1.0	2800-45000	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Focused	4.6	2800-10200	$\Delta E/ \sim 5x10^{-4}$	2.0 x 6.0	
VII-3	1.0	2800-45000	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Beam Line 0-0 (Lifetimes Port)	1.8	1-6	Bandpass $\geq$10A	4.0 x .4	Pulsed Visible

*Under construction
January 19, 1984

TABLE II-6

III MACHINE PHYSICS STUDIES

LOW EMITTANCE CONFIGURATION FOR SPEAR

An optical configuration has been designed for SPEAR which gives a horizontal electron beam emittance of $E_x = 13 \times 10^{-8}$ m-mrad at 3 GeV. This is about a factor of 3.5 smaller than the standard configuration and can significantly improve the quality of the photon beams from SPEAR. (See L.N. Blumberg and R. Z. Liu, SSRL Technical Note 83/01). This is achieved by stronger focusing, especially in the horizontal plane. The resulting betatron tunes are larger ($\nu_x = 7.2$, $\nu_y = 6.2$) compared to the standard values of $\nu_x = 5.27$ and $\nu_y = 5.16$.

As a further improvement, the new configuration gives a smaller value for the vertical beta function in the long straight section where wigglers and undulators are, or can be, installed. The stability of the particles in this lattice has been modelled using the program PATRICIA with satisfactory results. This high tune results in a horizontal betatron phase advance between the injection kickers larger than 180° which would make accumulation difficult if not impossible. The proper phase advance is restored by shunting the horizontally focusing quadrupoles between the kickers. After accumulation, the shunted current is reduced and all the quadrupole current adjusted such that the final symmetric configuration can be reached without changing the tunes.

This shunt and the magnet control were implemented and tested this fall. Just before going to press with this Activity Report, on February 8, 1984, a low current beam at 1.88 GeV was injected without accumulation in an intermediate configuration. The lifetime of this beam was over 2 hours and its emittance, E_x = [illegible] $\times 10^{-8}$ m-rad, was in good agreement with expectations for this energy.

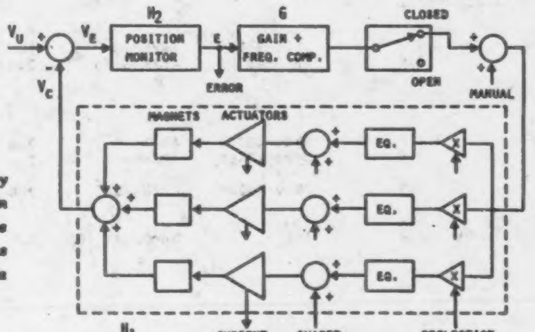
BEAM STEERING & STABILITY DEVELOPMENTS

Beam Steering

With a characteristic opening angle given by 1/γ, the synchrotron light beam is highly collimated in the vertical (~2 mm size at 20 m), and its alignment in a beam line is strongly dependent on the vertical electron orbit parameters (particularly slope) at the source point. A similar situation exists in the horizontal dependence direction for undulator and, to a lesser degree, for wiggler sources. Orbit control at each source point is required not only to steer collimated beams with submillimeter accuracy to experimental stations located some 20 meters away, but also to compensate for long and short term orbital fluctuations that translate to beam position instability. Sources of these fluctuations include long term orbital drift, SPEAR tune variations, mechanical vibration of ring magnets or other electron-optical components, electrical ripple on magnet power supplies, etc.

Each SSRL beam line is equipped with a beam position monitor and steering servo system for maintaining vertical position stability (Figure III-I). Horizontal steering is also provided for undulator and wiggler lines when necessary, but only in open-loop mode as horizontal position monitoring has not yet been implemented.

Figure III-1



Steering Servo System

Unsteered position V_u is corrected by deflection V_c to yield steered position V_e. Steering bump magnets can be shared between beam lines or used as independent correctors for SPEAR via the actuator summing points.

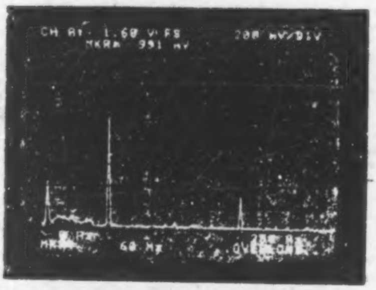
Independent steering for a beam line is accomplished by means of a three magnet orbital "bump" confined to an interval of the SPEAR ring containing the source point. The relative deflection strengths, or deflection ratios, of the dipole electromagnets must be adjusted to values dependent on the SPEAR tune to attain a compensated bump that minimizes orbit perturbations elsewhere in the ring, particularly at other source points and in the colliding beam regions. In general, a nominal electron orbit must be established using SPEAR-controlled corrector magnets to bring beams within the operating range of the steering systems.

The position monitor provides the center line reference for steering, producing an off-center error signal proportional to displacement that is used in the closed-loop system to maintain beam centering. A split anode helium ion chamber located near the experimental stations serves as a vertical monitor for each beam line. (On Beam Line VI, an in-vacuum photoelectron monitor located up stream of the mirror can be used when the line is in focused mode.) The ion chamber monitors have a beam position accuracy on the order of 10 microns when the upper and lower anode circuits are matched to .1%, and have a displacement sensitivity in the micron range. Originally, they were allotted a portion of beam in a dedicated steering port, but new non-interfering wide gap models have been installed directly in experimental branch lines (I-5, IV-1, VI-2, VII-1) and are presently used for steering. Since the accuracy and stability of steering adjustments are intrinsically limited by the performance of the position monitors, they are subject to on-going development.

Frequency analysis of the monitor's error signal reveals a beam noise spectrum typified by that for Beam Line III in Photographs III-2. (0 Hz - 250 Hz) and III-3 (0 Hz - 50 Hz). The exact components and amplitudes vary with time and with beam line. Components below 60 Hz are primarily related to small orbital oscillations induced by the mechanical vibration of magnets and their support structures. The predominant peak at 4.8 Hz is attributed to ground motion driving a fundamental torsional mode of the concrete magnet girders in the north and south SPEAR arcs (see following section). This peak corresponds to a vertical beam position "bounce" at the monitor which has an RMS amplitude in the tens of microns (microradian orbital oscillations), reaching peak values of ~ .1 mm, and is sufficient to degrade signal-to-noise ratios for many experiments at SSRL.

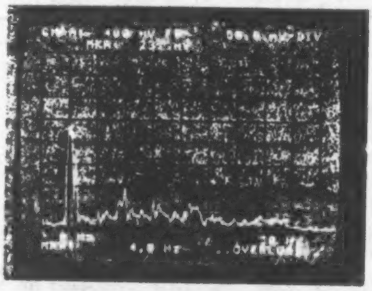
Higher frequency components occurring mainly at 60 Hz and at harmonics of 180 Hz are electrically induced, although the level of actual beam bounce at these frequencies has not been determined. They are caused in part by electrical noise in the sensitive monitor circuits, and there is evidence that a beam intensity modulation with an unrejected common mode signal is also present.

Photograph III-2



Representative beam noise spectrum (RMS), 0 Hz - 250 Hz, given by the BL IV position monitor error signal. The largest peak is at 60 Hz.

Photograph III-3

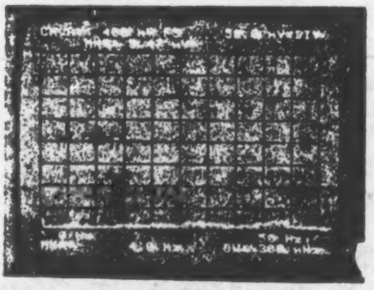


Beam noise spectrum (RMS), 0 Hz - 50 Hz. Components centered at 4.8 Hz are induced by mechanical vibration modes of magnet girders being driven by ground motion.

Until recently the steering system was not capable of significantly suppressing even the 4.8 Hz beam bounce. System bandwidth was limited by the use of resistive current shunts to set deflection ratios for the three series-driven bump magnets. The remotely programmable shunts enabled the reduction of DC and very low frequency beam line steering interaction, but this interaction became excessive at frequencies greater than a few hertz and imposed bandwidth restrictions for stable closed-loop operation. In addition, proper shunt adjustment was cumbersome and the system would not accommodate future closely spaced beam lines that must share the limited number of available steering magnets.

The deficiencies of the series-driven steering system have been largely overcome with the implementation of a parallel-driven system: that is, one that uses a separate current actuator for each steering magnet. Deflection ratios are set by appropriately scaling the feedback control signal to each of the three actuators associated with a beam line. Bump compensation can be maintained to a few hundred hertz, enabling a higher stable gain and bandwidth than previously realizable. Although the bandwidth is inherently limited by the solid iron-core magnet response and by eddy current attenuation in the walls of the SPEAR vacuum chamber, a 40 dB suppression of the 4.8 Hz oscillation is attainable (see Photograph III-4), rolling off to 6 dB at 60 Hz, when the system is properly tuned. In addition, shared magnet configurations for closely spaced beam lines are rapidly accomodated by means of control signal summing points for the actuators; they also enable the steering magnets to be used eventually as independent correctors for enhanced orbit control.

Photograph III-4



Noise spectrum, 0 - 50 Hz, with BL III steering system in closed-loop mode. The 4.8 Hz, component has been attenuated by a factor of 67.

The full power of this system will not be exploited until:

1) it is expanded to include horizontal steering and orbit control;
2) the control system is redesigned to incorporate computer control functions (such as AGC, deflection ratio control, optimal orbit control, etc.) based on real-time beam, lattice, and other steering system parameters and;
3) the position monitor system is improved for greater stability, noise immunity, and common mode signal rejection.

Beam line decoupling, orbit control, and position monitoring requirements will become more stringent as the number of closed-loop systems, and the demand for more stable beams by experimenters, increases.

Beam Stabilization

During the last half of 1983 some progress was made in understanding the origin of the "4.5 Hz beam bounce" and in reducing its magnitude. The following paragraphs briefly describe the highlights of the mechanical aspects of this work.

Previous work has shown convincingly that the 4.5 Hz vertical oscillation of the SSRL photon beams appears to originate in ground vibrations driven mostly by the large reciprocating hydrogen compressors which are used by the SLAC bubble chamber. As mechanical isolation of these compressors from the ground would be a formidable task, other alternatives were sought. This led to a vibration survey of the SPEAR storage ring components, using a sensitive seismometer and spectrum analyzer.

The vibration survey, in which the amplitudes and frequency spectra of the vertical motions of every quadrupole magnet in the ring were measured, showed two important facts. Firstly, the rms amplitude of the 4.5 Hz components of the vertical motions of many of the QD (vertically defocusing) quadrupoles fell in the range of 0.1 μm to 0.4 μm, large enough to be a possible cause of angular electron orbit deviations at 4.5 Hz consistent with the observed motions of the photon beam. Secondly, it was found that the large concrete girders (18 in number around the ring) which support the quadrupoles and bending magnets have, as their lowest-frequency fundamental mechanical vibration mode, a very weakly-damped torsional mode whose frequency is approximately 4.5 Hz (actual values include 4.38 Hz, 4.52 Hz, 4.56 Hz, 4.76 Hz, etc., depending on the particular girder studied). This strongly suggested that the structural properties of the support girders could be resulting in resonant mechanical amplification of the much lower amplitude (approx. 0.01 μm, rms) ground motion at 4.5 Hz.

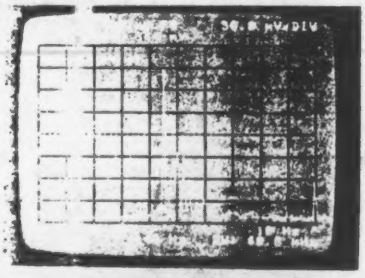
To test this hypothesis and possibly reduce the 4.5 Hz motion of the quadrupoles mechanically, a system of very robust (i.e., stiff) hydraulic jacks was designed and installed in the ring. The ten concrete girders exhibiting the largest amplitudes of motion at 4.5 Hz were each supported, at the antinode of the aforementioned torsional vibration mode, by separate hydraulic rams (between the underside of the girder and the ground) all connected to a single hand-operated hydraulic pump in the SPEAR control room. The vibration spectra were then studied with and without this hydraulic system activated, while beam was stored in the ring.

Photograph III-5 and III-6 are representative of the results of such tests. Photograph III-5 shows the spectrum of Fourier coefficients of the temporal record of the BL-VII position monitor difference signal, in the 0 to 10 Hz range, before the jacks were pressurized. The largest peak, at 4.48 Hz, is seen in the lower photograph (which was taken with the jack activated and providing an upward force of about 800 pounds) to be reduced by a factor of approximately 9. On the other hand the peak at 6.0 Hz has been increased (by a factor of about 5 in this case), indicating that the structure may have been altered so as to have a new vibration mode with a frequency around 6.0 Hz.

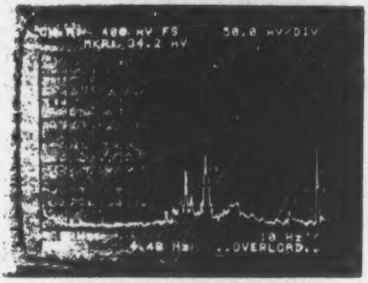
In summary, it appears fairly clear from this work that ground vibrations do cause the photon beam to vibrate, that the structural features of the storage ring components can and do exacerbate such vibrations by mechanical resonant amplification of this ground motion, that by appropriate modifications to these structures to eliminate certain offending modes the photon beam can be "quieted down" at discrete frequencies, but also that in so doing there is some risk of introducing new modes and corresponding increased beam bounce at other discrete frequencies. The electrical measures to be described below, based on a fast-responding beam steering system, appear to offer the significant advantages, relative to the mechanical vibration mode elimination techniques, of much larger noise reduction factors and continuous reduction across a broad range of frequencies.

Machine physics studies of the newly installed 54 pole wiggler were also carried out to determine its effect on stored beam (see Section V on Beam Line VI).

Photograph III-5



Photograph III-6



Spectra of Position Monitor Difference Signal, Beam Line VII, 10/31/86
(E = 1.88 GeV, I = 5 ma, Manual Steering)

Photograph III-5: without hydraulics
Photograph III-6: with hydraulics activitated
(Force approx. 800 lbs)

IV IMPROVEMENTS TO EXISTING FACILITIES

A. IMPROVEMENTS TO EXISTING BEAM LINES & EXPERIMENTAL STATIONS

X-RAY BEAM LINES

During the past six months a new beam line (VI) and a new experimental station (IV-1) have been added to SSRL's x-ray capabilities. Beam Line II has undergone a face lift and all beam lines are approaching a standard configuration of optical and electronic components.

Experimental Station IV-1 was funded by Simon Frazier University and installed in December, 1982. It was made available to users along with the other fully functional wiggler side stations, IV-3 and VII-3, in the spring of 1983. This station is squeezed in between III-4 and IV-2 and set-up space is very limited.

Beam Line VI is SSRL's new 54 pole wiggler end station. Because of its unique characteristics, details of this beam line can be found in a separate section of this report.

Station II-2 has been permanently focused to take full advantage of the excellent performance of its mirror and mirror mover system. Experimental Station II-3 has been permanently unfocused, has a one milliradian horizontal acceptance, and the same spectral qualities as I-5.

The mirror supports on Stations IV-2 and VII-2 have been modified. The experience of the fall 1983 run indicates a major improvement in mirror thermal stability.

Three diffractometers are now available at SSRL. The two-circle materials diffractometer has been dedicated to Station IV-3. The four-circle diffractometer (CAD-4) can be installed on either I-5 or II-2. The six-circle diffractometer (Huber) is dedicated to VII-2. A spectrometer support facility is being integrated into the x-ray staff shop.

As of March 1984, all x-ray lines, except VI-2, will be equipped with DEC PDP 11/34 computers, 2 RL01 disk drives and either a VI100 or LA120 terminal. This means software is completely interchangeable on all stations except VI-2. Also standard on all x-ray lines are water-cooled, double-crystal monochromators [Si(111) and Si(220) crystals available], precision entrance and exit slits, a long and a short ion chamber, a three channel voltage to frequency converter, and a triple digital voltmeter panel.

An encoded micrometer is scheduled for installation in the VII-3 monochromator for testing in January 1984. The new micrometer is part of the continuing effort to reduce monochromator sensitivity to external vibrations.

The beam line check-out procedure has matured in the past year. It is standard procedure to test the monochromator and table for accuracy and the data acquisition system for electronic problems before any experiment is allowed to go on-line. The beam line is calibrated and a comparative flux measurement is recorded.

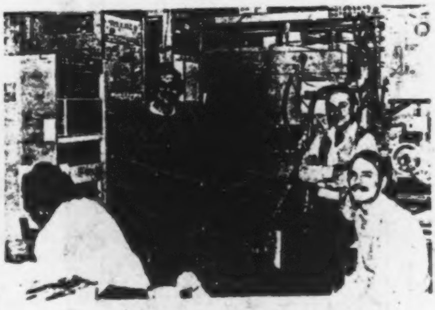


photo - H. Winick

Experimenters from Argonne National Laboratory and West Virginia University working on Station II-3.

photo - H. Winick

SSRL Operator, Joe Prazsl

VUV BEAM LINES

The work on the VUV and soft x-ray beam lines has continued to emphasize general improvements to existing experimental stations to increase monochromator reliability and make it easier for users to operate the systems. In terms of general improvements, interspace pumping systems have been added to all the experimental stations, standard NIM modules for pulse shaping are available on request and a build up of CAMAC, Keithley and NIM spares is underway. In addition, a set of electronics for the I_0 monitor is being added to each experimental station. The terminal and hardcopy capabilities on Beam Lines I and III are being standardized. Beam Line III is being rearranged to be serviced by VT-100 Terminals plus a Selanar graphics package which is compatible with existing software and allows the LA 120 (Decwriter) to be used for graphics hard copy. This should improve reliability and long term maintenance on this system. Beam Line I is now equipped solely with Tektronix 4025 terminals and hard copy unit.

The major improvement on the new Grasshopper has been the installation of an improved flip actuator which to appears to function well. This new actuator will no longer get "stuck" and provides more positive and reproducible seating of the grating holder. New holographic gratings and SiC Codling mirrors have been ordered for both Grasshoppers. This will give a total of three 1200 ℓ/mm gratings for both the old and new Grasshoppers as well as one each 300 ℓ/mm, 600 ℓ/mm and 1800 ℓ/mm gratings for the new Grasshopper. Jumbo has been improved extensively over the past six months. First, new control racks have been installed and the old ones rearranged to a more convenient configuration. A new I_0 section is being assembled for installation during January. The most significant improvement to Jumbo has been the installation of high accuracy encoders on the goniometer turn-tables. These encoders have an accuracy of 0.5 arc-second and are currently being used to characterize the monochromator crystals. So far, the effect of crystal heating on the Ge and quartz crystals has been studied and the data is being analyzed. When the crystal heating effects are eliminated by reducing the input power, the encoders can be used to get a measure of the monochromator's mechanical rigidity, stability and reproducibility. When these experiments were performed it was found that the monochromator linkages do not exhibit noticeable flexing and are reproducible. Therefore, once a model for the crystal heating is implemented, the new encoders may be able to be used to scan the monochromator without "max search."

Experimenters from EXXON and the University of Pennsylvania studying fragmentation of small molecules following soft x-ray absorption on the new Grasshopper (III-1) Line

photo - H. Winick

B. FACILITY IMPROVEMENT PROJECTS

CONVENTIONAL CONSTRUCTION

SSRL expansion continued throughout this last six months with the construction of another addition to Building 120. This recent expansion (approximately 2,900 sq. ft.) of the building will accommodate the future installation of new Beam Lines VIII & IX on the North Arc of the SPEAR storage ring. The addition was designed and constructed with the provision of adding a future second floor. This second floor will also provide the support for a rising beam line. This addition was one of the last projects to be funded by the National Science Foundation.

MIRROR COATING FACILITY

The Large Mirror Coating Chamber (LMCC) at SSRL has been completed. The mirrors for Beam Line VI and Station VI-1 were coated using this facility which is located at the Center for Materials Research on the Stanford University Campus.

Plans for this coming year include developing improved coating techniques and coating additional mirrors.

BIOTECHNOLOGY DEVELOPMENT PROJECTS

SSRL is an NIH Biotechnology Center which, in collaboration with DoE support, provides enhanced capabilities for biotechnology related experiments. Progress in major development projects during the past six months is summarised below.

SSRL Computer Facilities Improvements

The central VAX 11/780 has had many improvements. The most important is the addition of a 456 Mbyte fixed-disk RA81 mass storage device which has greatly increased the capability of on-line file storage. Physical memory has been increased to 2.5 Mbytes which allows more users to efficiently run programs simultaneously. The number of terminal ports has been increased to 32 and will soon be doubled to 64, thus giving a greater variety of locations for terminals.

A terminal room was built just outside the VAX room. There are seven terminals in the room for public access. Many of these are either VT125 or Selanar Tektronix emulation graphics terminals for use in data analysis. Several VAX terminal lines will be added to various beam line locations to aid in the convenient use of the on-line data analysis programs.

DECnet lines have been placed near several of the beam lines where the RSX EXAFS data acquisition package is most frequently used. These are slow (9600 baud) lines but have so far proved to be adequate for small data transfers. They have worked quite successfully with the on-line VAX data analysis package.

The SSRL standard RSX-11M EXAFS data acquisition package described in the 1982 Activity Report has proved quite popular. The package will allow the user to scan in motor steps, energy (eV), or in k-space and use up to 36 scaler inputs. Programs have been added for adding files together on-line, plotting on a second X-Y recorder, and plotting on a graphics terminal. Documentation is now available that describes how to use the RSX EXAFS programs.

EXAFS Data Analysis Package

SSRL now has its own, generally available, EXAFS data analysis package. The computer program is in essence the package put together by Don Sandstrom and his associates at Washington State University. It handles raw data from the data collection computers, and allows users to examine and manipulate the data through the initial stages of data reduction. It covers the translation to 'energy' space, correction of edge shifts, transformation to 'k-vector' space, and Fourier transformation and filtering. Users can even extract phase shifts from the data, and then, with a suitable choice of model compound, determine bond length changes. The package is very 'user friendly', allowing most of the input to be given using a graphics cursor. The original program has been extended to cover all the data formats currently being used at SSRL. Specifically, it will support the new RSX EXAFS data collection format.

All the EXAFS beamline computers can now be connected, via DECnet, to the central VAX computer. The analysis package can be told to operate upon data already present, or being collected at these experimental stations. This allows one to process spectra at the beamline, during a run. Users can now know within minutes if the quality of their data justifies further collection, or suggests abandoning the run to proceed with something else.

A Dedicated Rotation Camera Facility for Protein Crystallography

During the last eighteen months, we have designed and have essentially completed the installation of a dedicated rotation camera facility on a side station of the 8-pole wiggler Beam Line VII. The high intensity beam available from the wiggler is focused by x-ray optical elements in both the horizontal and the vertical planes. This doubly-focused beam should provide an extremely bright source of x-rays that will facilitate the collection of protein crystallographic data from:

(1) crystals with very large unit cells;
(2) crystals with very small dimensions and;
(3) crystals which are radiation sensitive.

It will also be possible to collect data very rapidly and to a higher resolution than with conventional sources. Since the energy of the beam is tunable, anomalous scattering data can be collected at elemental absorption edges.

The Beam Line VII steering monitor was modified to allow approximately 1.3 horizontal milli-radians of additional high intensity synchrotron x-radiation to be extracted. This created a second side station designated VII-1. (See Figure IV-1). This side station has been equipped with an experimental enclosure, which is the size of a small room, for radiation protection. The enclosure incorporates an interlocked system of swinging bars that will provide easy access to the experimental apparatus without requiring intervention by an SSRL operator.

A 19 cm long cylindrically bent triangular crystal monochromator has been installed and will function as the focusing element in the horizontal plane. This crystal has an asymmetric cut which increases the intensity of the x-ray beam and also reduces the distance between the monochromator crystal and the focusing point at minimum x-ray bandwidth (the "Guinier" position). The monochromator is followed by a 58 cm platinum coated fused-silica x-ray quality mirror which will be inclined to the incident x-ray beam to reject the higher energy harmonic components in the beam. The mirror will be bent to focus the approximately 0.17 milli-radians of beam in the vertical plane. A remotely controlled high-resolution TV camera, with a zoom lens, has been mounted inside the enclosure to simplify beam focusing and camera alignment.

An Enraf Nonius rotation camera, a backstop, a film carousel and a set of tantalum X-Y slits have been mounted on a 1 meter long optical bench, which is in turn mounted on an align-

ROTATION CAMERA FACILITY

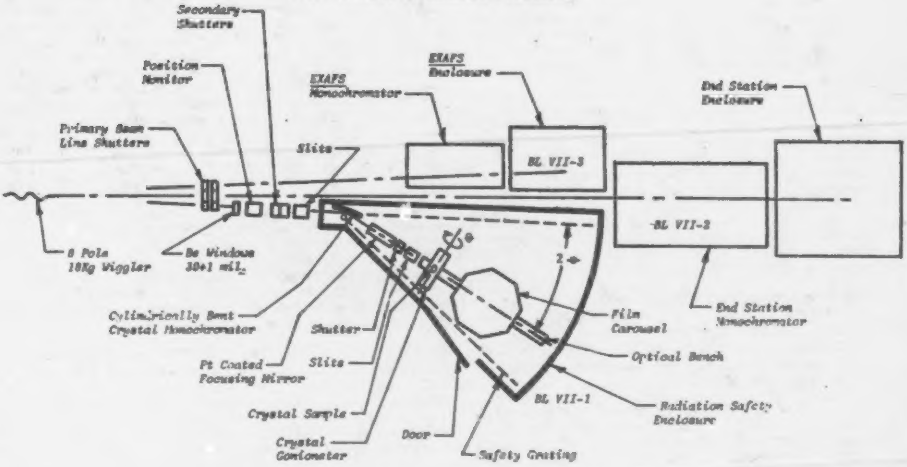

Secondary Shutters
Position Monitor
EXAFS Monochromator
EXAFS Enclosure
End Station Enclosure
Primary Beam Line Shutters
Slits
BL VII-3
BL VII-2
8 Pole 18Kg Wiggler
Be Window 30+1 mil
2
Cylindrically Bent Crystal Monochromator
Shutter
Film Carousel
End Station Monochromator
Pt Coated Focusing Mirror
Slits
Optical Bench
Crystal Sample
BL VII-1
Radiation Safety Enclosure
Crystal Goniometer
Door
Safety Grating

Figure IV-1

ment carriage. This carriage is mounted on a second optical bench. These optical benches permit the focal distance and distances between individual components to be easily changed. The second optical bench is pivoted below the monochromator crystal and can be rotated about a vertical axis so that the x-ray wavelength can be readily changed over a large range. This will provide an opportunity to collect anomalous scattering data at any one of a large number of elemental absorption edges. However, it is expected that the system will normally be set to a given x-ray wavelength (such as 1.5418 Angstroms or 1.08 Angstroms) for extended periods of time and will be used primarily for the rapid collection of high quality diffraction data to high resolution and for the investigation of smaller and also radiation sensitive crystals.

The motions of all the optical elements and of the rotation camera crystal phi axis and film carousel are under the control of a PDP 11/23 computer system through a CAMAC interface. We are currently developing control software for system alignment and data collection that will be flexible, convenient and very straightforward to use. The software system will also safeguard the beam line optics and other mechanical components against user input errors. Furthermore, it will provide the capability (a user option) of rotating the crystal phi axis at a speed determined by the incident x-ray flux, a normalization which makes the intensity of the recorded diffraction pattern independent of beam intensity fluctuations.

Sixteen flat film cassettes and four high resolution angled cassettes will be available for data collection. A number of cylindrical film cassettes and additional flat film cassettes will probably be purchased in the future depending on the demand.

An FTS systems crystal cooling device has been purchased and is currently being installed. This will provide temperature control at the sample position over the range -85°C to +100°C and to an accuracy of approximately 0.1°C, according to the manufacturer's specifications.

An Enraf-Nonius x-ray generator, with a sealed fine-focus Cu tube, is being installed about 20 feet away from the rotation camera. This generator will be fitted with a special collimator so that fiducial marks can be placed on the x-ray film packs after exposure. There will also be a precession camera available (on the second x-ray port) for pre-alignment of crystals, if desired.

A large darkroom (12' 6" x 11' 6") has been constructed for the rotation camera facility and is situated only about 50 feet away from the camera. Temperature controlled processing tanks, complete with N_2 burst capability, have been installed. There are a large number of wash tanks and three film driers. Ample bench and shelf space has also been provided. A film viewing area will be built shortly with a light box and a Supper circular film measuring instrument, etc.

SSRL will purchase x-ray film (either CEA reflex 25 or the new Kodak direct exposure film type SO-445) just prior to an experimental running period and keep the film refrigerated. The user would then be charged for the amount used. This will assure that fresh film is always available and will hopefully reduce the cost.

Crystal mounting equipment already exists in the biotechnology laboratory at SSRL, with a stereo microscope, Supper optical analyser, glassware and adequate bench space.

Since Beam Line VII-1 will be used exclusively by the rotation camera facility, the Proposal Review Panel approved, during its meeting of 18-19 June 1982, the request to permit access to the facility on a first come-first served basis. The proposed scheduling procedures are as follows:

1. Schedule two overlapping approved projects at a time.
2. Until a large backlog occurs, SSRL staff should retain the option of deciding whether preliminary data justifies an immediate assignment of time to collect a full data set.
3. Projects will be assigned an approved/ disapproved status and an advisory pilot, full data set status by the biology subpanel acting as follows:

   A one page proposal form will be mailed to all three biology sub-panel members. One member will coordinate phone responses from the other two. Unless strong objections are voiced, an approval will be telephoned to SSRL.

4. If a large backlog builds up, the PRP will want to assign priorities to proposals that involve collections of full data sets. However, pilot projects must continue to receive the rapid response outlined above.

Currently we have no plans to provide a film densitometering and processing facility at SSRL. This decision is based on the fact that there are a large number of regional facilities already in existence throughout this country and furthermore that there are not sufficient staff members here to adequately support such a facility.

After the system has been completed in the next few weeks, it will be thoroughly tested to check x-ray intensity, thermal loads on the beam line components, x-ray energy calibration, x-ray bandwidth calibration, beam focusing, mechanical stability, etc. If these tests go well, we hope to open the facility to outside users during or before the March 1984 dedicated running period.

Multi-Wire Area Detector System Developments

After several years of development at SSRL, a facility for anomalous scattering studies in protein crystallography is now operational and is permanently installed behind the EXAFS station on the unfocused Beam Line I. This facility incorporates a 5-circle diffractometer and a multi-wire area detector, both of which are under local computer control. During the past year we have continued to develop the hardware and control software of this facility for protein crystallographic structure determination using the phases derived from data collected at multiple x-ray energies. An online set of software documentation is provided to assist users during the operation of the system. Data images are processed on the local control computer and subsequent crystallographic analysis (such as the calculation and refinement of phases) are performed on a VAX 11/780 computer system.

The detector system has been used during the past year to investigate two protein structures and extensive sets of data have been measured from each, as outlined in the Experimental Progress Report for 651Bp. Data reduction software has been written and refined during the reduction of data collected earlier in the year. The resultant corrected intensities are currently being analysed.

Past mechanical problems with the beam line monochromator have been eliminated. During recent tests the energy repeatability was found to be well within acceptable limits. Improvements to the area detector system implemented over the past year include:

- Successful switchover to a Xe/CO_2 detector gas mixture from the previously used Ar/CH_4 mixture with consequent improvement in detector efficiency and data collection rates, particularly at higher photon energies.

- Addition of an FTS systems cooling device that provides temperature control at the crystal sample over the range -85°C to +100°C. Although this device has not yet been tested, the temperature can be maintained to an accuracy of 0.1°C according to the manufacturer's specification.

- Conversion of the computer control and analysis programs to run under the RSX-11M operating system. This has allowed network communication with the rest of the SSRL computer resources, and improved both the speed and flexibility of data handling. The addition of a 300 MByte disk to the local computer system results in an increase in the data handling rate and permits large scale rapid access to stored raw data images which was previously impossible. This simplifies the process of data collection and data analysis considerably.

- Development of computer programs for the determination and refinement of the sample crystal orientation, and of the physical parameters of the diffractometer and beam geometry upon which this depends. These are valuable because of the wide range of input beam energies at which data collection may be carried out (with consequent repositioning of the monochromator, diffractometer alignment carriage, detector, and x-ray mirror), and because of the desire to confirm sample crystal orientation as rapidly as possible in order to conserve beam time.

- Installation of a NaI fluorescence detector near to the sample crystal in the horizontal plane at 90° to the incident x-ray beam. This detector allows us to collect EXAFS scans of the sample crystal while it is mounted on the diffractometer. The x-ray energies of the absorption edges of bound anomalously scattering atoms in the crystal lattice depend on the local environment; in order to use the anomalous scattering effects for phasing it is thus important to calibrate the monochromator settings used during data collection to the absorption edge energies of the sample crystal itself. We have found that generally the signal-to-noise ratio is sufficiently high to provide excellent EXAFS scans in a reasonably short time period.

V NEW BEAM LINES AND EXPERIMENTAL STATION

BEAM LINE V

Beam Line V is being developed for photons in the soft x-ray range. Undulators are to be used as the radiation source and a single monochromator of the Rowland circle type will be followed by multiple experimental stations. The project is a collaboration between SSRL, Stanford University and the Xerox Palo Alto Research Center, with funding coming from the National Science Foundation, the Department of Defence and the Xerox Corporation. Plans for the beam line have been described previously in the 1982 and 1983 Activity reports. New developments for the period 4/83 - 12/83 are outlined below.

The Undulator: Two of SPEAR's four rf cavities were removed in the summer and PEP style klystrons installed for the two remaining cavities. The new klystrons allow SPEAR to reach 4 GeV with only two cavities and one of the two spaces released will be utilized for the Beam Line V undulators.

The specifications for the undulator section require that radiation be provided in the range 10 eV to > 1000 eV. After extensive modelling studies of the undulator, it has been decided that several different out-of-vacuum undulators will be mounted on a single mechanism. Each device is optimized for a particular tuning range and changing from one undulator to another will be possible during running time. Three new undulators will be built in addition to the existing 30 period SSRL device. Parameters for these undulators are shown in Table V-1 below.

In all cases permanent magnets ($Sm\ Co_5$) will be used and the magnetic arrangement will be that of the existing undulator, namely four magnetic orientations per period. The parameters chosen allow the fundamental of the undulator spectrum to be tuned from 16 - 1260 eV with SPEAR operating at 3 GeV. For photon energies between 10 and 50 eV, the off axis radiation from the 10 period device will be used.

Beam Transport: Conceptual design has been completed for all of the in-alcove components and detailed drawings are under way at present.

Power Filter: The extremely high flux from the undulator sources over portions of their tuning ranges, requires some method of filtering out unwanted power. A three-mirror filter will be placed in front of the monochromator and used when required. With the filter in place, the beam will undergo reflections of 2°, 4°, 2° before reaching the first element of the monochromator.

White Radiation Station: A one meter portion of the beam line before the monochromator has been reserved for experiments which take the radiation directly from the undulators. The quasi-monochromatic radiation from the undulators can be used for a range of experiments requiring high flux at low resolution.

Monochromator: The monochromator will be of the Rowland circle type with four gratings corresponding to four separate Rowland circle diameters on a single arm. The nominal grating parameters are summarized in Table V-2. Interchange between grating will be very straightforward, requiring the same set of motions as those used for scanning. To obtain high resolution at the higher photon energies, very accurate rotations and translations must be made. A sensitivity analysis has shown that in regions of the operating range angles must be reproducible to about one arc-second and positions to within about one micron. A laser interferometer will be used to monitor position and angle and will be an integral part of the monochromator.

Table V-2

NOMINAL GRATING PARAMETERS			
GRATING ANGLE [Deg]	ROWLAND CIRCLE [m]	RULING DENSITY [l/mm]	WORKING RANGE [eV]
2	10	1200	229 - 1500
4	5	1200	88 - 350
10	2	600	7 - 150
20	1	600	7 - 50

Table V-1

Period length [cm]	18	12	7.7	6.1
Approx. No of Periods	10	15	24	30
Minimum Gap [cm]	3.0	3.0	3.0	3.0
Tuning range* of E [eV]	16 - 420	84 - 640	360 - 1020	800 - 1260

*Data is for 3.0GeV; divide energies by 4 for 1.5GeV. Low energy cutoff is set by minimum gap and by specifying a total power allowed at the optics; high energy cutoff corresponds to an undulator parameter K = 0.5.

The sensitivity of the optical elements to incident power has also been examined in detail. The major effect on the resolution and throughput of the beam line occurs when heating of the gratings changes their effective radius of curvature. Calculations of the power densities radiated by the undulators over their scanning ranges have been carried out and combined with heat flow studies for the optical elements. As a result it has been decided to limit the scanning range of the undulators so that no more than 40 w/cm or 40 w total power are incident on the Codling mirror. In addition, both the gratings and the Codling mirror, which receives a much higher flux density, will be water cooled in order to protect and stablize these elements.

BEAM LINE VI

This beam line, a collaboration among EXXON, LBL and SSRL, began operation near the end of this reporting period. The radiation source is a 2 m long, 54 pole permanent magnet wiggler of the hybrid design. The wiggler and the beam line were described in detail in previous SSRL Activity Reports and in the Proceedings of the Hamburg Conference on Instrumentation for Synchrotron Radiation Research [see E. Hoyer et al, Nucl. Instr. & Meth. 208, 117-125, (1983)]

Installation of the wiggler, its mover control system and almost all the alcove beam line components was completed during the summer, 1983 shutdown. Component installation outside the alcove and completion of beam line and end station electronics and control systems continued after the start of operation in October. To avoid possible interference with SPEAR operation during the start up, the wiggler magnet gap was initially set at 12 cm (corresponding to a peak field of only .006 T) and the vacuum chamber aperture was set at 1.8 cm to provide full aperture for injected beams.

Tests of Wiggler Effects on Stored Beam: Once SPEAR became operational, tests of the effects of the wiggler and vacuum chamber on the stored beam were carried out, starting on October 28, 1983. Vacuum chamber apertures as small as 6 mm at 1.8 GeV and 9 mm at 3 GeV have so far been tested with no adverse effect on stored beam lifetime. Magnet gaps as low as 12 mm (corresponding to a peak field of 1.2 T) have also been successfully tested at low electron energy and current (to keep radiated power levels low).

Trim coils at each end of the wiggler are used to null the field integral through the wiggler and thus to eliminate, or make negligible, possible orbit distortions due to the wiggler. The currents required for this were determined experimentally at several magnet gap settings using the 24 electron beam position monitors in SPEAR. Some differences were found between trim coil currents determined this way and the settings determined by magnetic measurements. It wre also found that sometimes the stored beam lifetime decreased (e.g., from 15 hours to 5 hours) as the wiggler gap was closed. The lifetime could be restored by increasing the strength of rotated quadrupole fields in SPEAR. This effect will be studied more in the future.

Tests of the Beam Line: Installation of beam line components, control systems and shielding outside the alcove was complete enough to bring an unfocused beam on to the SSRL experimental floor on December 14, 1983. The layout of the beam line outside the alcove is shown in Figure V-3. A feature of the line that is different from most other SSRL x-ray lines is the location of the hutch shutters downstream of the monochromator. This elimates the need for water cooling on these shutters and keeps the beam on the first crystal during access to the hutch, eliminating unnecessary thermal cycling of this crystal.

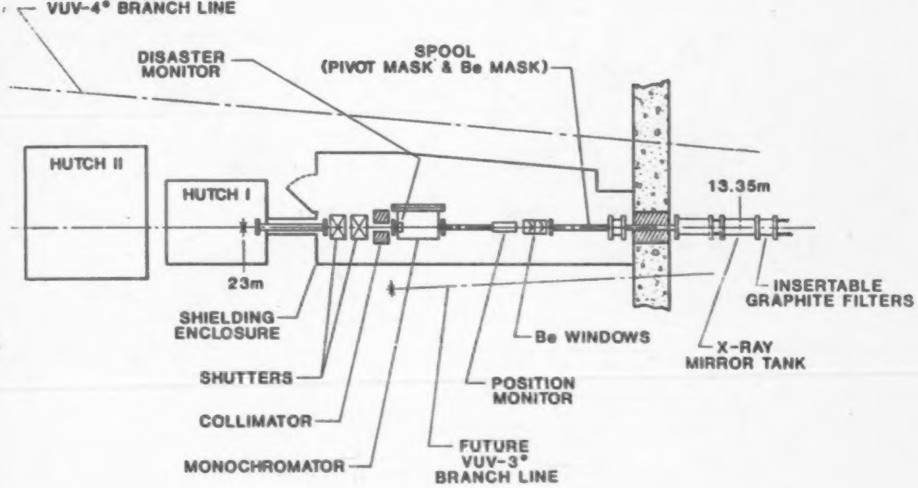
The beam was brought through the Be windows and the split ion chamber position monitor (which is at 18.8 m and may be remotely adjustable vertically) onto the first silicon crystal of the two-crystal monochromator. The beam could be steered vertically to strike the first crystal at the correct place. The color photograph in the front of this report shows the beam passing through the He system and striking the first crystal.

Position sensitive signals were observed on the split ion chamber and also observed on an in-vacuum photo-electron position monitor located at about the 7.5 m point. This in-vacuum position monitor can be electrically biased and remotely adjusted vertically to center it on the beam. However, neither of these features were ready for use in the initial tests. It is intended to use the in-vacuum position monitor when the line is operated in focused mode. Tests of focused mode operation are planned for early in 1984. Either position monitor can be used in a feedback system to stabilize the beam position. This feedback system will be put into operation in January, 1984. Both position monitors exhibit the desired linear response to variations in steering current, with about a 30-fold greater sensitivity on the in-vacuum monitor.

On December 15, 1983, the end station electronics and interlock systems were completed and a monochromatic, unfocused beam was brought into the hutch. From then until December 22 a variety of spectral measurements were made during normal SPEAR dedicated operation (3 GeV, up to 100 mA stored current) and with the wiggler peak field at 0.19 T and 0.3 T. At these rather low fields the device operates in the undulator mode [$K = 0.934\ B_o(T)\ l_u(cm) = 1.24$ and 1.96 respectively] and the quasi-monochromatic peaks of high harmonics could be observed clearly. The fundamental peak is at about 700 eV and 400 eV respectively so that the fundamental and first few harmonics do not penetrate the 0.5 mm total Be window thickness.

End Station Electronics: The Beam Line VI end station electronics and components they control have a familiar x-ray beam line theme. Due to the uniqueness of this beam line there are, however, some distinguishing departures from the norm.

Figure V-3


FUTURE
VUV-4° BRANCH LINE
DISASTER MONITOR
SPOOL (PIVOT MASK & Be MASK)
HUTCH II
HUTCH I
13.35m
23m
SHIELDING ENCLOSURE
SHUTTERS
COLLIMATOR
MONOCHROMATOR
Be WINDOWS
POSITION MONITOR
FUTURE VUV-3° BRANCH LINE
X-RAY MIRROR TANK
INSERTABLE GRAPHITE FILTERS

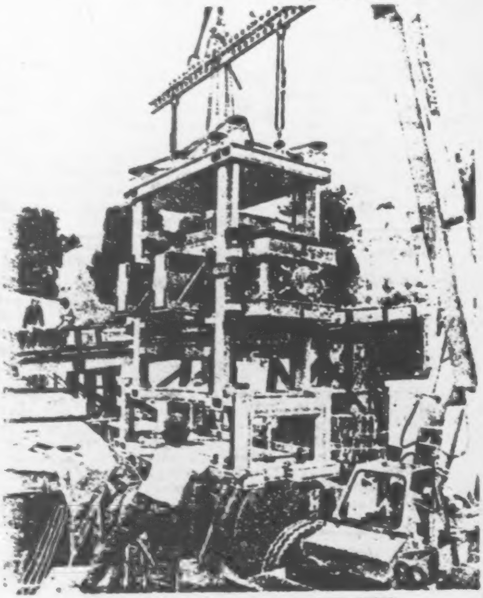
BL VI END STATION COMPONENTS

The removable focusing mirror has a new type of controller. Changes in the mirror focus are achieved by turning a single knob clockwise or counterclockwise for the exact motion (example tilt or translation) desired. Due to the potential thermal loads there are both hard and soft limits which are set to match running conditions of the wiggler. The mirror slits are four encoded wedges which are placed independently in front of the mirror to achieve the desired collimation and resolution.

The core of the data acquisition system is a DEC PDP 11/24 computer. The computer is intrinsically the same as a DEC PDP 11/34 which is standard on all other x-ray lines; in principle, software developed for another line will work here. The exception is that the machine makes use of RL02 disk drives and an automatic bootstrap feature. In addition to the PDP 11/24 and RL02 disk drives, the computer system is equipped with a Kennedy variable density tape drive and a multi-pen Nicolet plotter.

Future Operation of the Beam Line - Thermal Limits: By the end of the year the wiggler had operated in a mode (0.3T, 3 GeV, 100 mA) in which the total radiated power was about 100 W. This already exceeds the total radiated power that would be produced during typical colliding beam operation (1.85 GeV, 15 mA) with the wiggler at 1.2 T. This confirms our expectations that the beam line can operate at such high fields during most parasitic operation. At 1.85 GeV the spectrum would have a critical energy of 2.7 KeV and the 54 poles would produce very high flux out to 10-15 KeV.

photo by N. Cox



54 POLE WIGGLER BEING INSTALLED INTO SPEAR

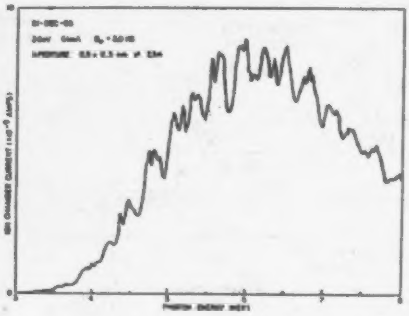
FIRST MONOCROMATIC LIGHT IN BEAM LINE VI

In dedicated operation we aim to reach 1.2 T also. At this field and with normal dedicated running conditions (3 GeV, 100 mA) the wiggler radiates 1.6 KW. Although this is 16 times larger than the values already achieved at 0.3 T, because of the larger horizontal divergence, the power density is up by only a factor of 4 from the already achieved levels. Calculations of thermal stresses on in-vacuum beam line components indicate that we can operate up to about 0.5 T with the beam line as presently configured and up to 1.2 T after the installation of certain components (particularly in-vacuum graphite filters and a Be Window mask assembly) that are now in fabrication.

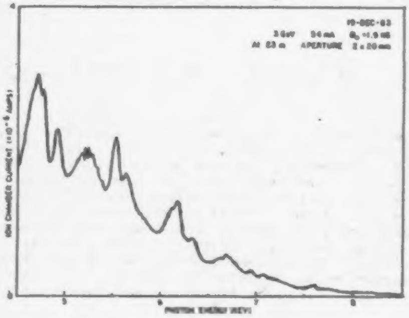
During routine operation the wiggler parameters will be controlled by the SPEAR operator via the SPEAR computer. This will assure that, during injection, the vacuum chamber gap is open adequately for efficient accumulation and also that, at high electron energy, radiated power levels will not exceed the capability of beam line components. Programs to accomplish this are now being written by SLAC computer programmers. The main concern is to keep thermal stress on the Be windows below calculated safe limits. The absorbed power in the Be windows depends on several factors (electron energy and current, wiggler field and graphite filter thickness).

As a backup to the computer control of wiggler power levels a "disaster monitor" is included in the beam line. This is a 1" x 4" x 4" can filled with He gas at 50 PSI pressure. It is located behind the crystal monochromator and aligned to block a possible incoming white beam but not the vertically displaced monochromatic beam. During normal operation of the beam essentially no radiation strikes this monitor. In the unlikely event of failure or absence of the first monochromator crystal and very high power level in the beam, pressure sensors on the disaster monitor will cause the line to close and, if necessary, dump the stored beam rapidly via a new, fast-acting, rf interrupt. This rf interrupt is also used in the event of a vacuum failure on the beam line to protect the fast valve which could be damaged in a fraction of one second under high power beam conditions.

CURRENT OBSERVED IN A 12 cm NITROGEN-FILLED ION CHAMBER



CURRENT OBSERVED AT 3 GeV, B_0 = 3.0 kG



CURRENT OBSERVED AT 3 GeV, B_0 = 1.9 kG

EXAMPLES OF
SPECTRA
TAKEN WITH
54 POLE WIGGLER

BEAM LINES VIIIW & VIIIB

The development of these beam lines is a collaborative effort involving investigators from the University of California campuses (UC), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), Sandia National Laboratory (SNL) and SSRL. Responsibility for the construction of these beam lines rests with LLNL and UC, with the cooperation of SSRL. Beam Line VIIIW will be a wiggler line, and Beam Line VIIIB will be a bending magnet line.

Present plans for the VIIIW wiggler call for an 18-pole device with a fixed vacuum gap. Radiation from the wiggler will be split by mirrors and potentially will feed three branch lines: a straight-through x-ray branch and two soft x-ray branches fed by approximately 4 degree reflections. The x-ray beam line will have an double-crystal monochromator that should cover the range from 4 to 50 keV photon energies. The decision about what type of monochromator to use on the first soft x-ray branch line will be made after more data become available on the new devices just now being commissioned at various synchrotron radiation sources around the world. The second soft x-ray branch line will be held open for future development.

Beam Line VIIIB will have two branches: a straight-through section and an 18 degree vertically deflected branch. The non-deflected branch will be used as a white-light source and a port for the development of monochromators and optics. A torodial grating monochromator (TGM) optimized for the photon-energy region from 10 eV to 100 eV will be the active element in the 18 degree branch line.

At present, the beam lines, the insertion device, and the monochromators are being designed. Conventional construction on the beam line alcove will be completed in the summer of 1984, with both beam lines scheduled for installation on SPEAR in the summer of 1985.

18° EXPERIMENTAL STATION

This "windowless" branch line on Beam Line III will provide VUV photons in the range 5 - 169 eV with good resolution in a small spot size. Full implementation of the line will allow gas-phase (as well as UHV) experiments to run in a windowless fashion. To date, the main support structure for the monochromator is complete and is to be installed in the summer of 1984. A major portion of the vacuum components will be installed at that time as well. The first monochromatized beam is expected in 1985. The 18 degree line is now affiliated with the Center for Advanced Materials (CAM) at LBL.

VI FUTURE DEVELOPMENTS

SSRL ENHANCED PHOTON FLUX FACILITY (SEPFF)

In the fall of 1982, SSRL was invited by the Lawrence Berkeley Laboratory to join in the Center for Advanced Materials (CAM) proposal, specifically to upgrade the x-ray research capabilities of SSRL. The invitation was accepted, and a tentative scope-of-work, based on earlier plans, was quickly established for the November, 1982 DoE construction review, and for the subsequent April, 1983 construction review. In May, 1983, the SEPFF Project Director was appointed, and by June the project scope evolved to its present state.

The SEPFF project embodies a number of subprojects intended to improve and extend the research capabilities of the Stanford Synchrotron Radiation Laboratory. The centerpiece of this project is an undulator beam line on the PEP electron-positron storage ring, which will produce an x-ray beam whose spectral brilliance in the wavelength region of 1 A will be unsurpassed by all other man-made x-ray sources. (Figure VI-1) The second major technical project will be a new beam line on the SPEAR storage ring, dedicated to x-ray scattering research, and utilizing a novel in-vacuum wiggler as source magnet. The SPEAR storage ring will be improved in three important ways: the machine horizontal emittance will be reduced by a significant factor (3.5); the beam stability will be improved significantly (a factor of 10 or more at 6 Hz.); and the capability of injection during the annual 3-4 month LINAC downtime will be developed. Finally, three separate buildings will be constructed to house the shop, laboratory, and office space required to accommodate the rapid expansion of the laboratory, and to house the PEP beamline and experimental area.

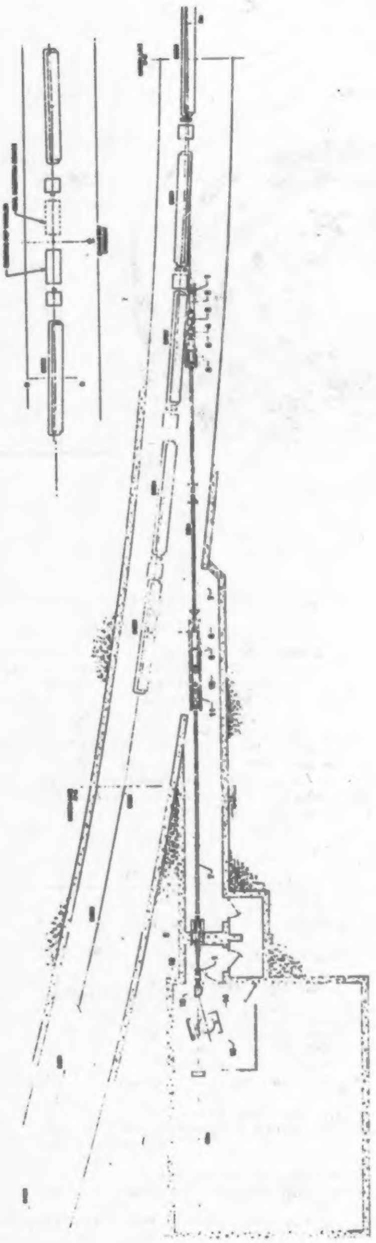
The planned funding for the project has exhibited several gyrations since the original proposal of $4.1 M construction funding in FY 1984. At the time of writing, $940 K has been appropriated for SEPFF, subject to a final review by the Surveys and Investigations staff of the House Appropriations Committee. If these funds are released early in 1984, construction of the PEP building will proceed in the summer of 1984, and the technical components will be installed in the summer of 1985. In the meantime, $80 K of R&D funds are being applied to the design of the state-of-the-art technical components of the PEP beam line. Total construction funding for this project is 12.6 K over a 3 year period. Progress is also being made on the emittance reduction program and the beam stabilization program, through machine physics and engineering studies. Finally, SLAC is proceeding with the construction of the off-axis electron injector, and in principal it will be possible to have summer injection into SPEAR in 1985.

PLANNING FOR SSRL 6 GEV STORAGE RING

As mentioned in the May, 1983 Activity Report, considerable thought has been given to the provision of "next generation" synchrotron radiation sources by the SSRL staff. Work in this area has actively continued over the past six months. A project leader has been appointed and with the aid of the New Rings Planning Group concrete design parameters are being formulated.

With the successful operation of wigglers and undulators in SPEAR and storage rings in other laboratories it was clear that the new ring should be designed so as to allow the use of many such devices at their optimum performance.

In order to reach photon energies of at least 20 KeV in the fundamental harmonic of the radiation spectrum from an undulator, the particle beam energy has to be at least 6 GeV. Since a high energy ring is not optimized for VUV and soft x-rays, the possibilities of providing a 2 GeV ring on top of the 6 GeV ring, or of rebuilding SPEAR as a low energy, low emittance, high current ring, are being considered. Since a new 2 GeV ring would have the same large circumference as the high energy ring it would allow a very flexible beam dynamics lattice. In particular, very long insertions (about 50 m or more) could be implemented for experiments and developments of FEL's or micro-beam bunching techniques to produce coherent radiation or special lattice arrangements to produce and investigate the stability of extremely short bunchs on the order of one picosecond. Figure VI-2 shows our present view of the general facility. The preliminary parameters of the rings are listed in Table VI-3. The characteristics from different sources are compiled in Tables VI-4 to VI-6.



SSRL BEAM LINE I
ON PEP

7-5-83

1. ISOLATION VALVE
2. FIXED MASK
3. MOVEABLE MASK
4. FAST VALVE
5. COLLIMATOR
6. INJECTION STOPPERS
7. DRIFT TUBE
8. POSITION MONITOR
9. HORIZ. & VERT. SLITS
10. MIRROR TANK
11. SHUTTERS
12. GRAPHITE FILTERS
13. MONOCHROMATOR
14. BERYLLIUM WINDOW
15. EXPERIMENTAL END-STATION

Figure VI-1

Figure VI-2

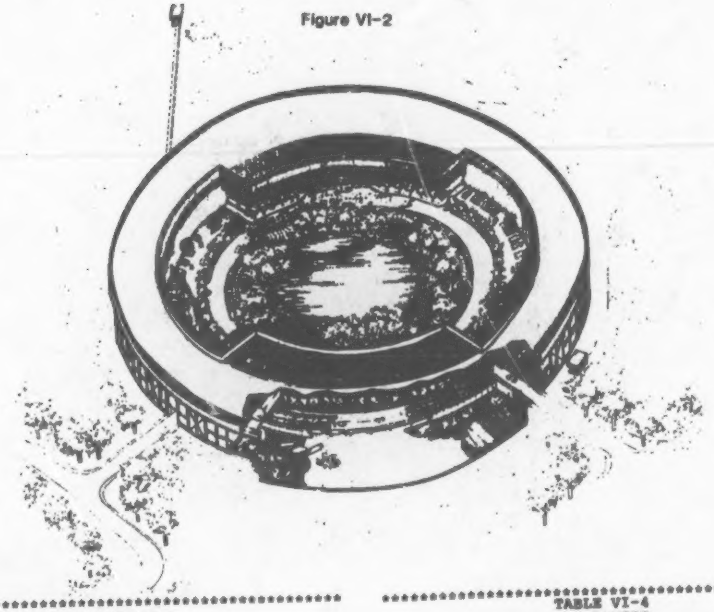


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TABLE VI-3

STORAGE RING PARAMETERS

(Tentative)

Ring		I	II
Energy	E(GeV)	2	6
Circumference	C(m)	536	536
Orbital Period	T_o(nsec)	1800	1800
Bending Radius	ρ (m)	19.1	19.1
Field	B(kG)	3.5	10.5
Beam Emittance			
no. coupling (K=0)	ε_{xo}(radm)	$21\text{x}10^{-9}$\*	$5.8\text{x}10^{-9}$
opt. coupling (K=50%)	ε_x(radm) ε_y(radm)	$16.8\text{x}10^{-9}$ $4.2\text{x}10^{-9}$	$4.6\text{x}10^{-9}$ $1.2\text{x}10^{-9}$
Beam Current			
per bunch	I_b(ma/bunch)	2.6	11.3
total	I_{tot} (ma)	200	100
Beam Lifetimes			
Touschek	T_t(h)	20	20
Coulomb	T_c(h)	20	20
Total	T (h)	10	10
Bunch Length**	σ_t(psec)	100	100
Average Vacuum	p(Torr)	$3\cdot10^{-9}$	$5\cdot10^{-9}$

*)a smaller beam emittance is possible for a reduced beam intensity

**)a smaller bunch length is possible at a reduced beam intensity or for a larger beam emittance

****

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TABLE VI-4

UNDULATORS

The beam parameters in the undulator sections have been adjusted for minimum beam divergence to maximize spectral brillance. The minimum gap size is determined by the aperture needed to get a 20 hour lifetime due to Coulomb scattering of beam particles on the residual gas atoms. This is also the effect that requires an average vacuum of 10^{-9} Torr. Occasionally it is possible to reduce the gap even more if useful. The penalty is a reduced beam lifetime: $T \sim G^2$;

Ring		I	II
Energy	E(GeV)	2	6
# of Undulator Sections	N_u	10	10
Length	L_u(m)	4.0	4.0
Beam Size	σ_x; σ_y(μm)	780;190	410;100
Beam Divergence	$\sigma_{x'}$;$\sigma_{y'}$(μrad)	22	11
Fund. Line Width for a 100 Period Undulator (N=100) divided by γ	$1/(\gamma\sqrt{N})$	$26\text{x}10^{-6}$	$9\text{x}10^{-6}$
Minimum Gap Free for Particle Beam	G_x(mm) G_y(mm)	35 10	9 5.5
Highest Fundamental Photon Energy	ε_p(keV)	1	20

****

* * *

TABLE VI-5
WIGGLERS

In the wiggler sections the beam parameters were chosen to produce a small spot size.

Ring		I	II
# of Wiggler Sections	N_w	20	20
Length	L_w(m)	2.0	2.0
Beam Size	$\sigma_x;\sigma_y$(μm)	450;100	90;40
Beam Divergence	$\sigma_x';\sigma_y'$(μrad)	40;20	50;30
Minimum Gap Free for Particle Beam	G_x(mm)	21	2.0
	G_y(mm)	12	2.0
Critical Photon Energy			
B_w = 20 kG	ϵ_c(keV)	5.3	47.5
B_w = 40 kG	ϵ_c(keV)	10.6	95.0

* * *

* * *

TABLE VI-6
BENDING MAGNETS

For some special applications one might want to make use of the large fan of synchrotron radiation from bending magnets. Where this is desirable one might choose the magnetic field parameters at the source point within a large range. Especially one can use shorter and stronger magnets than the nominal magnets but to some extent it is also possible to use weaker magnets.

Ring		I	II
Energy	E(GeV)	2	6
Nominal Bend Magnets			
Radius	ρ (m)	19.1	19.1
Field	B(kG)	3.5	10.5
Crit. Photon Energy	ϵ_c(keV)	0.92	24.9
Stronger Bend Magnets			
Radius	ρ (m)	3.3	10.0
Field	B(kG)	20	20
Crit. Photon Energy	ϵ_c(keV)	5.3	47.5

* * *

The first design concept was published at the National Accelerator Conference in Santa Fe (An All Wiggler and Undulator Synchrotron Radiation Source, H. Winick, H. Wiedemann, I. Lindau, K. Hodgson, K. Halbach, J. Cerino, A. Bienenstock, R. Bachrach, IEEE, NS, Vol. 30, 3097-9, No 4, August 1983) and a first special New Rings Workshop (New Rings Workshop, SSRL Report 83/02) to discuss the scope and desired performance of the new ring was held in July 1983 at Stanford. An additional workshop for machine aspects is being planned for June 25-29, 1984.

THE STANFORD X-RAY RADIATION LABORATORY (SXRL)

In a collaboration with a group headed by J. Madey at the Stanford campus, SSRL provides support for the design and construction of the SXRL, a 1 GeV storage ring (Design Study of a Free Electron Laser Storage Ring, H. Wiedemann, Stanford University, HEPL-TN-80-8). This ring is designed primarily for Free Electron Laser experimentation. The design of the ring, however, also allows the installation of up to four insertion devices in four 3 m long straight sections for the local community interested in the use of soft x-ray and VUV synchrotron radiation (Figure VI-7). A third component in the use of this ring will be experiments dedicated to the development of accelerator physics as well as hands-on training of graduate students in accelerator physics.

This ring provides a unique opportunity for this kind of training since it is not a national facility and is, therefore, much more flexible in its operation than other facilities can be. Since there are too few accelerator physicists in the United States the opportunity provided by this ring should help considerably.

Construction of this facility will begin in 1984.

FUTURE PEP SYNCHROTRON RADIATION SOURCES

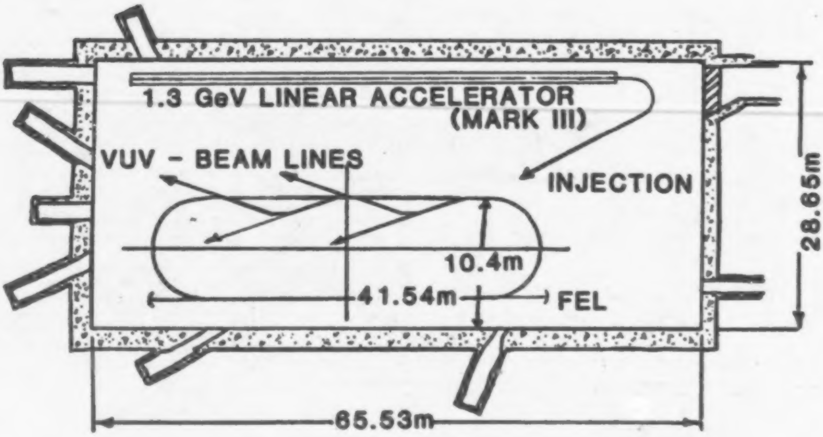
Members of the SSRL Machine Physics Group have begun preliminary thinking about how to implement additional insertion devices on the PEP storage ring beyond those in the symmetry straights. Of particular interest is the possible use of an interaction region (IR) if it were not in use for a high energy detector.

The PEP interaction regions are housed in large (20 m x 20 m) experimental halls centered on straight sections which are approximately 120 m long.

Although there are several variations, the basic idea is to deflect the electron beam by a few degrees horizontally as it enters the IR straight, through an undulator, and then restore it to its original orbit. The synchrotron radiation from the undulator would shine into an experiment in the IR hall. A similar "chicane" on the positron side is also possible. (See Figure VI-8.)

The characteristics of the synchrotron beam are similar to those of the PEP Beam Line Facility which is described above. The details of the electron transport system and the effect of such a chicane upon the colliding beam operation of PEP will require considerable study. No specific plans exist for further development of the concept at this time.

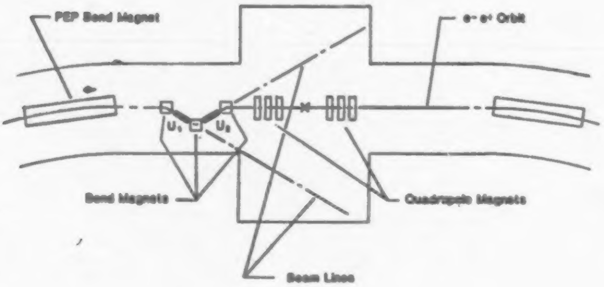
Figure VI-7


1.3 GeV LINEAR ACCELERATOR
(MARK III)
VUV - BEAM LINES
INJECTION
10.4m
41.54m
FEL
28.65m
65.53m

SXRL STORAGE RING FOR FEL EXPERIMENTATION AND FOUR SOFT X-RAY/VUV BEAM PORTS

Figure VI-8

X-RAY UNDULATOR BEAM LINE
IN A PEP INTERACTION REGION


PEP Bend Magnet
e- e+ Orbit
U1
U2
Bend Magnets
Quadrupole Magnets
Beam Lines

VII SSRL ADVISORY PANELS AND USERS ORGANIZATION

PROPOSAL REVIEW PANEL

A main task of the Proposal Review Panel is the review and rating of scientific proposals to SSRL based largely on reports obtained from outside (non-panel) referees. The panel met June 17th 1983 at SSRL and rated the new proposals which had been received in March, 1983. The panel will hold its next meeting at SSRL in January 1984.

As of December 31, 1983, SSRL had received a total of 865 proposals of which 196 are presently active.

The Proposal Review Panel meets twice yearly, generally in June and January. Deadlines for receipt of proposals for full consideration at the next meeting are the first of September and the first of March of each year.

The current panel members are:

Biology Sub-panel

Charles Cantor, Columbia University
(Chairperson)
Wayne Hendrickson, Naval Research Laboratory
William Orme-Johnson, MIT

Materials Sub-panel

Boris Batterman, Cornell University
Alex Bell, UC Berkeley
Denis McWhan, Bell Laboratories
David Turnbull, Harvard University

VUV Sub-panel

Bernd Crasemann, University of Oregon
Charles Fadley, University of Hawaii
Warren Grobman, IBM Watson Research Center

SCIENCE POLICY BOARD

The Science Policy Board reviews all aspects of SSRL operation, development and plans for the future. It reports to Stanford University President Donald Kennedy. The Board met once during this reporting period, on May 17th and 18th, 1983. The members at the time of the meeting were:

H. Frauenfelder, University of Illinois
(Chairperson)
Wm. Brinkman, Bell Laboratories
D. A. Shirley, Lawrence Berkeley Laboratory
W.D. Phillips, Washington University
H. Mark, NASA

After the May meeting the decision was made to expand the Board by adding a sixth member. The term of Dr. Phillips expired with the last meeting and the newly appointed member of the Board is: P. Wolff, MIT. In addition, a Machine Physicist will be asked to become a member of the Board.

SSRL USERS ORGANIZATION

Members of the Executive Committee of the SSRLUO were appointed at the Tenth Annual SSRL Users Group Meeting as follows:

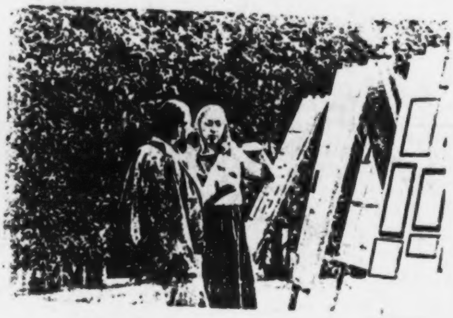
David Moncton, BNL (Chairperson)
Jim Allen, Xerox PARC (Vice-Chairperson)
Daryl Crozier, Simon Fraser University
Don Sandstrom, Washington State University
Rick Stulen, Sandia National Laboratory
John Barton, LBL (Student Representative)
Michael Seul, Stanford (Student
Representative)
Earl Skelton, NRL
Stanley Williams, UCLA
Mel Klein (LBL) (Ex Officio)
Katherine Cantwell, SSRL

The Users Organization Executive Committee meets periodically throughout the year to consider and advise on matters pertinent to user interests at the Laboratory.

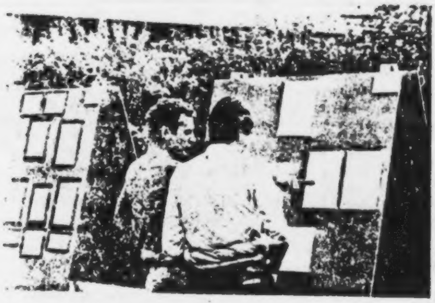
TENTH ANNUAL SSRL USERS GROUP MEETING

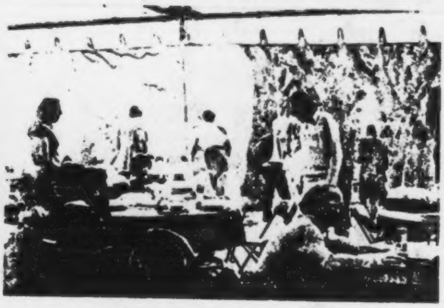
The Users Group Meeting this year had a special emphasis on the 10th Anniversary of the Laboratory. The SSRLUO Executive Committee is responsible for organizing the Users Group Meeting jointly with a representative of the SSRL Scientific Staff. The 10th Annual SSRL Users Group Meeting was held October 27 and 28, 1983 at SSRL. Approximately 190 people were in attendance. The program for the meeting and the authors' abstracts are available as SSRL Report Number 83/03.

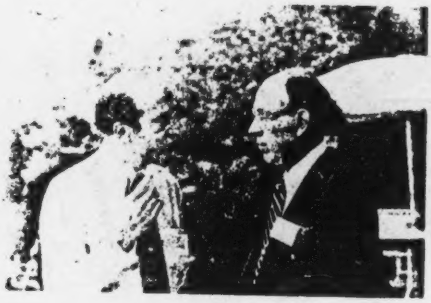
Co-Chairpersons for the meeting were David Moncton for the Users Organization and Piero Pianetta for the SSRL Scientific Staff. Reports on individual experiments were presented in poster sessions.

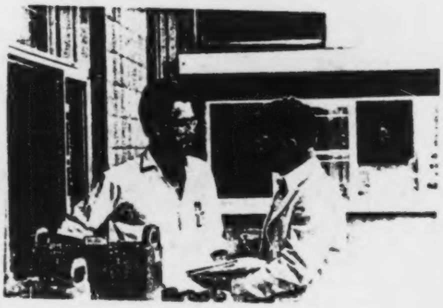


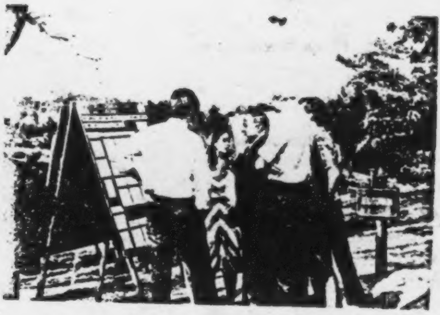
10th ANNIVERSARY USERS MEETING











Polarized

VIII SSRL ORGANIZATION

The chart on the following page depicts the organization of SSRL as of January, 1984.

The SSRL administration is divided into six areas each headed by a senior staff member. These are: X-ray, VUV, Biotechnology, Machine Physics, Operations & Engineering and Administrative Services.

Reponsibility for the each experimental station and piece of facility equipment is assigned to a staff scientist. The charts below detail these assignments as well as responsibilities for major SSRL Development Projects.

SSRL

CHART OF RESPONSIBILITIES

BRANCH LINE	RESPONSIBLE SCIENTIST
BL I-1 (4° VUV)	P. PIANETTA
BL I-2 (8° VUV)	P. PIANETTA
BL I-4 (CURVED CRYSTAL)	W. WARBURTON
BL I-5 (EXAFS I)	G. BROWN
BL II-2 (X-RAY)	G. BROWN
BL II-3 (X-RAY)	G. BROWN
BL II-4 (X-RAY)	G. BROWN
BL III-1 (4° VUV)	P. PIANETTA
BL III-3 (2° VUV)	P. PIANETTA
BL III-4 (3° X-RAY)	P. PIANETTA
BL IV-1 (WIGGLER)	G. BROWN
BL IV-2 (WIGGLER)	G. BROWN
BL IV-3 (WIGGLER)	G. BROWN
BL VII-1 (WIGGLER)	P. PHIZACKERLEY
BL VII-2 (WIGGLER)	G. BROWN
BL VII-3 (WIGGLER)	G. BROWN
LIFETIMES PORT (90° VUV)	TO BE DETERMINED

INSTRUMENTATION/FACILITY RESPONSIBILITIES

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HUBER SYSTEM: G. BROWN
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UNDULATOR: H. WINICK
BEAM LINE STEERING: H. WINICK

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ROTATION CAMERA - P. PHIZACKERLEY

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PEP BEAM LINE - G. BROWN/R. BOYCE
PEP BUILDING - G. BROWN/A. GOLDE
SCATTERING BEAM LINE - G. BROWN

PROJECTS IN INITIAL STAGES

BEAM LINE VIII, BEND MAGNET - P. EBERT (LLNL) & S. WILLIAMS (UC)
SSRL LIAISON - R. TATCHYN

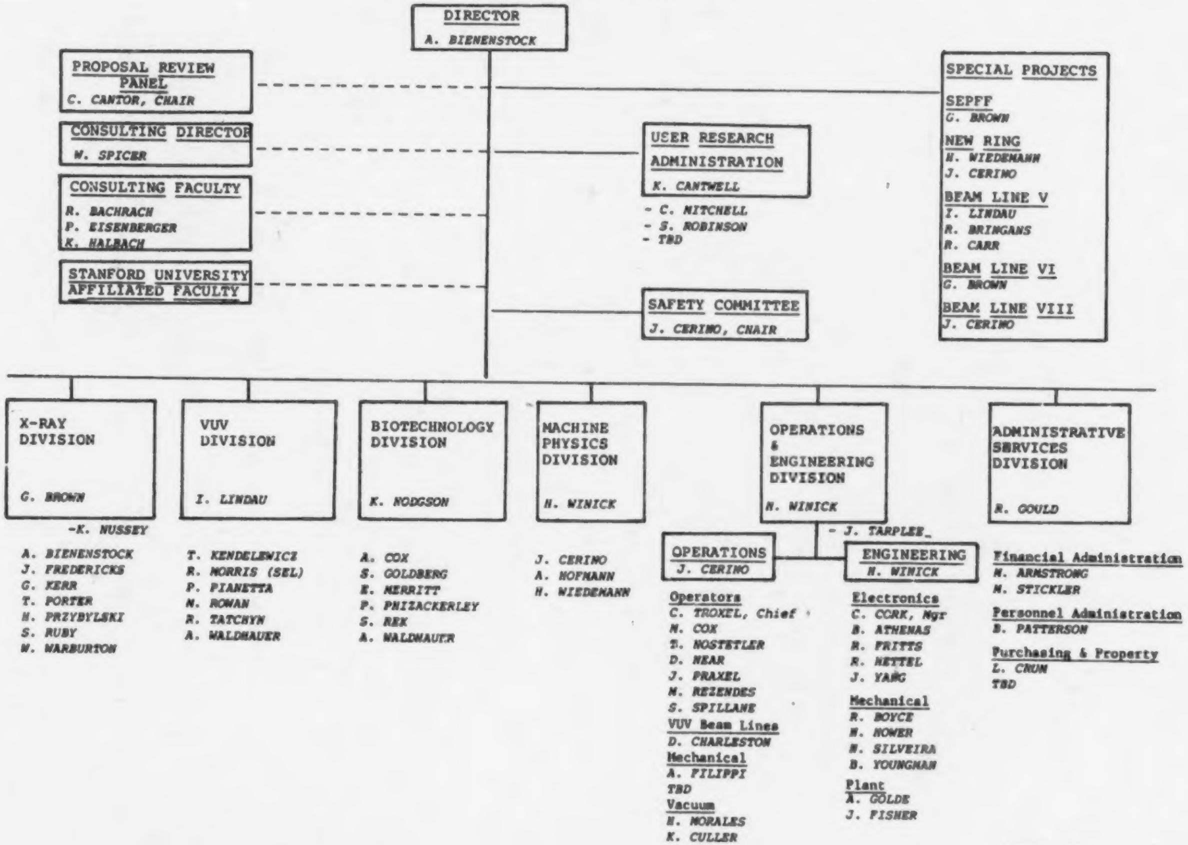
BEAM LINE VIII, WIGGLER - P EBERT (LLNL) & A. MARADUDIN (UC)
SSRL LIAISON - J. CERINO

MODIFICATION OF BEAM LINE IV FOR ANGIOGRAPHY -
G. BROWN/R. BOYCE

NEW RING - H. WIEDEMANN/J. CERINO
18 DEGREE LINE - D. LINDLE (LBL)
P. PIANETTA - SSRL LIAISON

NOTE: RESPONSIBLE PEOPLE ARE DENOTED SCIENTIST/ENGINEER.

STANFORD SYNCHROTRON RADIATION LABORATORY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H. WINICK
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C. CORK, Mgr
B. ATHENAS
R. FRITTS
R. HETTEL
J. YANG
Mechanical
R. BOYCE
H. HOWER
H. SILVEIRA
B. YOUNGMAN
Plant
A. GOLDE
J. FISHER
ADMINISTRATIVE SERVICES DIVISION
R. GOULD
Financial Administration
M. ARMSTRONG
M. STICKLER
Personnel Administration
B. PATTERSON
Purchasing & Property
L. CRUM
TBD

JANUARY 1984

IX EXPERIMENTAL PROGRESS REPORTS

These reports are submitted by Experimental Spokespersons as a summary of their activities during the period April 1, 1983 - December 31, 1983.

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X THESES BASED ON RESEARCH AT SSRL

The following list is a partial compellation of Ph.D theses based on experimental research at SSRL. We would appreciate receiving additions.

YEAR/STUDENT	INSTITUTION	TITLE/ADVISOR
1984		
R.S. Weber	Stanford University	"Structure and Reactivity of Platinum Clusters Supported on Y-Type Zeolites" (advisor - M. Boudart)
G.D. Meitzner	Stanford University	"Characterization of Gold/Y-Zeolite and its Catalytic Activity in the H_2 - O_2 Reaction" (advisor - M. Boudart)
1983		
P.M. Stefan	Stanford University	"A Photoemission Study of the Electronic Structure and Surface Chemical Properties of Tungsten Carbide and of a Carbonized Tungsten Model Surface for Tungsten Carbide" (advisor - W.E. Spicer)
A.N. Mansour	N. Carolina State	"X-ray Absorption Studies of Silica-Supported Platinum Catalysts" (advisor - D.E. Sayers)
J.G. Tobin	U.C. Berkeley	"Dimensionality and Its Effects Upon the Valence Electronic Structure of Ordered Metallic Systems" (advisor - D.A. Shirley)
C. Marques	Washington State U	"Thermal Motion of Surface Atoms in Silica Supported Platinum and Iridium Catalyst Clusters: An EXAFS Spectroscopy Study" (advisor - D.R. Sandstrom)
P.R. Findley	U.C. Santa Barbara	"Optical Properties of PbF_2 and $PbCl_2$ at High Temperatures" (advisor - W.C. Walker)
M.R. Antonio	Michigan State	"Extended X-ray Absorption Fine Structure Studies of the Iron-Molybdenum Cofactor of Nitrogenase, the Three-Iron Ferredoxin II of Desulfovibrio Gigas, and of Synthetic Molybdenum- and Tungsten-Iron-Sulfur and Iron-Sulfur Model Systems (Part I) and Intercalation of Tetrathiafulvalene into Iron Oxycholoride (Part II)" (advisor - H. Eick)
G.B. Stephenson	Stanford University	"Early-Stage Phase Separation in Amorphous Solids: A Time-Resolved SAXS Study" (advisor - A.I. Bienenstock)
J.M. Tranquada	Univ. of Washington	"X-ray Absorption Studies of Solids at High Pressure" (advisor - E. Stern)
D. Stearns	Stanford University	"Early Photo Luminescence Decay in Amorphous Hydrogenated Silicon" (advisor - A.I. Bienenstock)
S. Laderman	Stanford University	"Structural Studies of Amorphous Semiconductors Containing Transition Metals" (advisor A.I. Bienenstock)
M.S. Co	Stanford University	"X-ray Absorption Spectroscopy of Hemocyanin and Hemerythrin" (advisor - K.O. Hodgson)
S.D. Conradson	Stanford University	"X-ray Absorption Studies of the Molybdenum Site on Nitrogenase" (advisor - K.O. Hodgson)
R. Miake-Lye	Stanford University	"Anomalous X-ray Scattering as a Probe of Biological Structure" (advisor - K.O. Hodgson)

C.C. Parks	U.C. Berkeley	"The Auger Decay Mechanism in Photon Stimulated Desorption of Ions from Surface" (advisor - D.A. Shirley)
D.B. Goodin	U.C. Berkeley	"The Local Structure of Manganese in the Photosynthetic Apparatus and Superoxide Dismutase: An X-ray Absorption Study" (advisor - M. Klein)

1982

M.G. Durrett	Rice University	"Study of KrCl/Kr$_2$Cl Excited State Kininetics Using Synchrotron Radiation Excitation" (advisor - G.K. Walters)
J.G. Nelson	U.C. Los Angeles	"Angle Resolved Photoelectron Spectroscopy Applied to the Determination of the Electronic Structure of Ge(001) 2x1" (Master's Thesis - R.S. Williams)
M.L. Shek	Stanford University	"Electronic Structure of Platinum-Copper Surfaces and Chemisorption of Carbon Monoxide" (advisors - I. Lindau, W.E. Spicer)
P.R. Skeath	Stanford University	"Chemical Bonding Phenomena of Column 3 and 5 Adsorbates and Fermi Energy Stabilization Mechanisms on GaAs (110)" (advisors - I. Lindau, W.E. Spicer)
M.H. Hecht	Stanford University	"Synchrotron Radiation Measurements of Subshell Photoionization Cross Sections: Techniques and Applications" (advisor - I. Lindau)
S.-J. Oh	Stanford University	"Resonance and Relaxation Effects in Photoemission Spectroscopy" (advisor - I. Lindau)
S.M. Brennan	Stanford University	"Surface EXAFS of Sulphur on Nickel" (advisor - A.I. Bienenstock)
R.O. Tatchyn	Stanford University	"The Introduction and Development of a New Method for Measuring the Optical Constants of Metals in the Soft X-ray Range" (advisor - I. Lindau)
P.A. Heiney	M.I.T.	"Phase Transitions of 2D Atomic and Molecular Crystals" (advisor - R.J. Birgeneau)
D.H. Rosenblatt	U.C. Berkeley	"High Resolution Electron Energy Loss Spectroscopy and Photoelectron Diffraction Studies of the Geometric Structure of Adsorbates on Single Crystal Metal Surfaces" (advisor - D.A. Shirley)
J.E. Pollard	U.C. Berkeley	"Photoelectron Spectroscopy of Supersonic Molecular Beams" (advisor - D.A. Shirley)
S.H. Southworth	U.C. Berkeley	"Atomic and Molecular Photoelectron and Auger Electron Spectroscopy Studies Using Synchrotron Radiation" (advisor - D.A. Shirley)
K. Jackson	Stanford University	"Photoion Fluorescence Polarization: A Study of Molecular Ionization Dynamics" (advisor - R.N. Zare)
V. Yachandra	Princeton University	"EXAFS Studies of Carbonic Anhydrase and Resonance Ruman Spectroscopy of Iron-Sulfur Proteins" (advisor - T. Spiro)

1981

J.M. Fine	Washington State U	"Structure and Stoichiometry in Highly Concentrated Aqueous Solutions of CuBr$_2$" (advisor - D.R. Sandstrom)
C.-Y. Su	Stanford University	"Photoemission Studies of the Interaction of Oxygen with Solid Surfaces" (advisor - I. Lindau)

D.L. Weissman	Stanford University	"Oxygen Chemisorption and Water Synthesis on Palladium and Palladium-Gold: A Study by Thermal Desorption and Photoemission" (advisor - W.E. Spicer)
R.F. Davis	U.C. Berkeley	"Angular Distribution and Atomic Effects in Condensed Phase Photoelectron Spectroscopy" (advisor - D.A. Shirley)
F. Kutzler	Stanford University	"Electronic Structure Calculations of Germanium, Molybdenum Chromium and Febium Compounds Predicted K and L Edge Absorption Spectra" (advisor - K.O. Hodgson)
1980		
B. Bunker	Univ. of Washington	"An X-ray Absorption Study of Tetrahedral Semiconductors" (advisor - E. Stern)
J.M. Lornston	Univ. of Delaware	"Characterization of Pt/Al_2O_3 Catalysts by Extended X-ray Absorption Fine Structure" (advisors - J.R. Katzer/J.M. Schultz)
P.H. Fuoss	Stanford University	"Structural Studies of Amorphous Materials Using X-ray Anomalous Scattering" (advisor - A.I. Bienenstock)
D.J. Trevor	U.C. Berkeley	"Photoelectron Photoion Molecular Beam Spectroscopy" (advisor - D.A. Shirley)
S.D. Kevan	U.C. Berkeley	"Normal Emission Photoelectron Diffraction: A Now Technique for Determining Surface Structure" (advisor - D.A. Shirley)
R.V. Taylor	U.C. Santa Barbara	"Matrix Spectroscopy of Rare-Gas Oxides and Sulfides" (advisor - W.C. Walker)
P. Frank	Stanford University	"The Biochemistry of Transition Metals: Copper, Vanadium, and Iron" (advisor - K.O. Hodgson)
1979		
M. Breining	Univ. of Oregon	"Precision Determining of Atomic Level Energies by Absorption Spectrometry with Synchrotron Radiation" (advisor - B. Crasemann)
F.A. de Parente	Univ. of Oregon	"Measurement of the Inelastic Scattering Cross Section of Neon with Synchrotron Radiation" (advisor - B. Crasemann)
T.D. Bonifield	Rice University	"Time Resolved Spectroscopy of Krypton and Xenon Molecules Excited by Electron Impact and by Monochromatic Synchrotron Radiation" (advisor - G.K. Walters)
J.N. Miller	Stanford University	"Photoemission Studies of Adsorption and Oxidation of Selected Metals and Semiconductors" (adviser - I. Lindau)
D.T. Ling	Stanford University	"Angle-Integrated and Angle-Resolved Photoemission Studies of Chemisorption on Copper and Copper/Nickel" (advisors - I. Lindau, W.E. Spicer)
K.A. Mills	U.C. Berkeley	"The Determination of Electronic States in Crystalline Semiconductors and Metals by Angle-Resolved Photoemission" (advisor - D.A. Shirley)
D.R. Denley	U.C. Berkeley	"Determination of Morphology and Electronic Structure in Solids with 20-1000 eV Radiation" (advisor - D.A. Shirley)
E.D. Poliakoff	U.C. Berkeley	"Time-Resolved Spectroscopy Using Synchrotron Radiation" (adviser - D.A. Shirley)

M.G. White	U.C. Berkeley	"Photoelectron Spectroscopy of Heavy Atoms and Molecules" (advisor - D.A. Shirley)
R.A. Rosenberg	U.C. Berkeley	"Studies of Electron Correlation in the Photoionization Process" (advisor - D.A. Shirley)
T.D. Tullius	Stanford University	"Structures of Metal Complexes in Biological Systems: EXAFS Studies of Blue Copper Proteins, Xamtjome Oxidase and Vanadocytes" (advisor - K.O. Hodgson)
1978		
C.M. Garner	Stanford University	"Surface and Interface Studies of Oxygen on Silicon, III-V Heterojunctions, Schottky Barriers" (advisors - I. Lindau, W.E. Spicer)
J.C. Phillips	Stanford University	"Crystal Structure Determination Using Synchrotron Radiation" (advisor - K.O. Hodgson)
P.W. Chye	Stanford University	"Photoemission Studies of the Oxidation of and Schottky Barrier Formation on GaSb, InP, and GaAs" (advisor - W.E. Spicer)
S.P. Cramer	Stanford University	"Chemical Application of X-ray Absorption Spectroscopy-Nitrogenase and Cytochrome P-450" (advisor - K.O. Hodgson)
T. Eccles	Stanford Universtiy	"X-ray Absorption Studies of Hemocyanin" (advisor - K.O. Hodgson)
R.S. Williams	U.C. Berkeley	"Angle-Resolved Photoelectron Spectroscopy Applied to the Determination of the Surface Electronic Structure of Crystalline Metals" (advisor - D.A. Shirley)
P.S. Wehner	U.C. Berkeley	"Valence Band Photoemission Studies of Clean Metals" (advisor - D.A. Shirley)
1977		
G.E. Ice	Univ. of Oregon	"Measurements of X-ray Scattering Cross Sections of Hydrogen and Helium with Synchrotron Radiation" (advisor - B. Crasemann)
P.A. Pianetta	Stanford University	"Photoemission Studies of Solids Using Synchrotron Radiation" (advisor - W.E. Spicer)
S.H. Hunter	Stanford University	"A Structural Study of Amorphous Copper-Arsenic Triselenide Alloys using EXAFS" (advisor - A.I. Bienenstock)
G.R. Apai II	U.C. Berkeley	"Photoemission Studies of Clean and Adsorbate Covered Metal Surfaces Using Synchrotron and UV Radiation Sources" (advisor - D.A. Shirley)
1976		
K.Y. Yu	Stanford University	"Photoemission and Thermal Desorption Studies of the Adsorption of Simple Molecules on Transition Metals and Alloys" (advisor - W.E. Spicer)
F.R. McFeely	U.C. Berkeley	"Relaxation and Cross Section Effects in Valence Band Photoemission Spectroscopy" (advisor - D.A. Shirley)
1975		
P.E. Gregory	Stanford University	"Ultraviolet Photoemission Studies of the Surface States and Properties of the (110) Gallium Arsenide Surface, and of the Oxidation of Cesium" (advisor - W.E. Spicer)

B.M. Kincaid	Stanford University	"Synchrotron Radiation Studies of K-edge X-ray Photoabsorption Spectra: Theory and Experiment" (advisor - S. Doniach)

1974

C.A. Ashley	Stanford University	"Extended X-ray Absorption Fine Structure" (advisor - S. Doniach)

XI ACTIVE PROPOSALS

As of December 31, 1983 there were 196 active SSRL proposals. Proposals remain active for two years after their initial rating by the Proposal Review Panel. Since October 1974 SSRL has received a total of 865 proposals. In September 1979 SSRL began accepting proposals for scientific programs. The 90 active program proposals are indicated by a p after the panel letter. The Spokesperson for each proposal is underlined and their institution shown in parentheses. The letter suffix appended to the proposal number indicates the sub-panel of the Proposal Review Panel to which the proposal is assigned: Materials (M), Biology (B) or Vacuum Ultra-Violet (V).

No.	Received	Experimenters	Title
100 PRT	9/7/83	E.D. Crozier W. Alberding A.J. Seary K.R. Bauchspiess R. Ingalls J. Whitmore P. Viran F.W. Lytle R.B. Greegor (Simon Fraser University)	X-ray Absorption Studies of Disordered Systems
456Bp	7/5/79	E.B. Hughes E. Rubenstein H.D. Zeman D.C. Harrison R. Hofstadter (Stanford University)	Iodine Dichromography with Monochromatic X-ray Beams for Angiography
471Mp	8/29/79	D.R. Sandstrom F.W. Lytle (Washington State University)	Investigation of Support Effects Chemisorption, and Surface Disorder in Catalysts by X-ray Absorption Spectroscopy
474Mp	8/30/79	J.H. Sinfelt G.H. Via F.W. Lytle G. Meitzner J. M. Brown (Exxon)	Structural and Electronic Properties of Dispersed Metal Catalysts
489Mp	8/31/79	R.L.Ingalls E.D. Crozier J.E. Whitmore J.M. Tranquada (University of Washington)	X-ray Absorption Studies of Materials Under High Pressure
490Bp	8/31/79	E.A. Stern W.W. Parson (University of Washington)	X-ray Absorption Studies of Metalloproteins
509Mp	9/5/79	P.H. Fuoss W. Warburton M.H. Grabow (Bell Laboratories)	Anomalous Scattering Techniques and Their Application to Disordered Systems
518Bp	9/6/79	J.K. Blasie S. Gruner A. Scarpa L. Herbette K. Rothschild (University of Pennsylvania)	Time-Resolved Structural Studies of Integral Membrane Proteins

No.	Received	Experimenters	Title
523Vp	9/7/79	D.A. Shirley A.C. Baca C.C. Bahr J.J. Barton T.C. Ferrett P.A. Heimann L.E. Klebanoff D.W. Lindle G. Liu E. Paparazzo M. N. Piancastelli S.W. Robey M. Schulz A.E. Schach Von Wittenau L. Terminello L. Wang (University of California-LBL)	VUV and Soft X-ray Spectroscopy of Gases, Solids and Surfaces
528Vp	9/7/79	P.H. Citrin J.E. Rowe F. Comin (Bell Laboratories)	SEXAFS Studies of Adsorbates on Single Crystal Semiconductors
543Mp	2/19/80	H.L. Yakel C.J. Sparks (Oak Ridge National Laboratory)	Determination of Site Occupation Parameters in 3d Transition Metal Phases
559Bp	3/4/80	R.C. Elder K. Tepperman (University of Cincinnati)	EXAFS of Gold-Based Drugs used to Treat Rheumatoid Arthritis
562Mp	3/5/80	E.A. Stern J. Budnick (University of Washington)	Many-Body and Chemical Effects in EXAFS
564Mp	3/10/80	P.H. Fuoss A. Fischer-Colbrie (Bell Laboratories)	Application of X-ray Reflection-Diffraction Techniques to the Study of Disordered Interfaces
582Vp	8/21/80	R. Bachrach R. Bringans (Xerox PARC)	Relationship of Atomic and Electronic Structure of Semiconductor Surfaces and Interfaces
598Mp	9/2/80	M. Boudart M. Samant R.A. Dalla-Betta (Stanford University)	In Situ Characterization of Platinum Fuel Cell Working Electrocatalysts
599Vp	9/2/80	M.L. Knotek G.M. Loubriel R.H. Stulen J.A. Kelber T.A. Michalske (Sandia National Laboratories)	Photon-Stimulated Desorption and Auger Spectroscopy
608Mp	9/4/80	P. Eisenberger S. Brennan P.S. Sande (Exxon)	Reflection Diffraction Scattering Program
611Mp	9/16/80	T.W. Barbee W.K. Warburton J. Underwood (Stanford University)	Layered Synthetic Microstructure Characterization and Research Program
614Vp	9/16/80	I. Lindau M.L. Shek G. Rossi P. Jupiter W.E. Spicer (SSRL-Stanford University)	The Electronic Structure of Metal Surfaces, and Overlayers on Metals

No.	Received	Experimenters	Title
615Mp	9/18/80	F. Lytle R. Greegor (Boeing Company)	Investigation of Atomic and Electronic Structure of Glass
616Vp	9/22/80	I. Lindau B. Pate G. Rossi B. Petro J. Silberman P.J. Jupiter S. Eglash W.E. Spicer D. Laser P. Mahowald J. Nogami J.J. Yeh (SSRL-Stanford University)	The Electronic Structure, Chemistry, and Fermi Energy Pinning of Semiconductor Surfaces
623Mp	10/21/80	S.K. Sinha P. Dutta P.M. Horn (Exxon)	High-Resolution Diffraction Studies of Carbon Tetrafluoride Monolayers Physisorbed on Graphite
631Mp	2/27/81	J. Stohr R. Jaeger (Exxon)	Photon Stimulated Ion Desorption: Mechanistic Studies and Application to Surface Chemistry and Crystallography
632Bp	3/2/81	B. Chance L. Powers C. Kumar Y. Ching J. Valentine (University City Science Center)	Structure-Function Relationships in Cytochrome-c Oxidases, Related Oxidases Peroxidases and Models
634B	3/16/81	W. Hendrickson R.P. Phizackerley C.W. Cork W.E. Love W.E. Royer (Naval Research Lab)	Anomalous Scattering Crystallography of Lamprey Hemoglobin
639Mp	3/4/81	J.B. Kortright W.K. Warburton A.I. Bienenstock (Stanford University)	Structural Studies of Amorphous Mo-Ge Alloys
641Bp	3/9/81	D.H. Templeton L. Templeton (University of California-LBL)	Anomalous Scattering Measured by Single Crystal Diffraction
647Mp	3/17/81	G.P. Huffman F.E. Huggins L.J. Cuddy F.W. Lytle R.B. Greegor (US Steel Corp Res. Lab)	EXAFS Investigation of Problems of Interest to the Steel Industry
650Mp	3/23/81	R.H. Martinson W.S. Rothwell R.L. Gorman R.W. Holsinger (Lockheed Palo Alto Res. Lab)	Dynamic Small Angle Scattering Experiments on Polymeric Materials

No.	Received	Experimenters	Title
651Bp	3/24/81	R.P. Phizackerley K. Hodgson C.W. Cork E.A. Merritt L.M. Amzel W.A. Hendrickson J.L. Smith D.H. Templeton L.K. Templeton M. Hatada C. Ogata G. Tomlinson Sung-Hou Kim B. Hedman (SSRL-Stanford University)	Protein Crystallographic Structural Studies Using Anomalous Scattering
652Vp	3/30/81	R.S. Bauer H.W. Sang A. Katnani (Xerox-PARC)	Imperfections and Formation of Semiconductor Interfaces
662Mp	8/31/81	E.A. Stern Y. Yacoby (University of Washington)	Development of Modulation Techniques with Applications to Ferroelectrics
669M	9/1/81	M.P. Scott J.R. Carruthers R.S. Smith (Hewlett Packard)	Real Time X-ray Topography of Oxygen Precipitation in Silicon
670Bp	9/1/81	A. Thompson J. Jaklevic T. Hayes (University of California-LBL)	Development of a Scanning X-ray Microprobe
678Mp	9/1/81	J. Wong F.W. Lytle R.L. St. Peters C. L. Spiro (General Electric)	Trace Element Sites in Coal and Other Fossil Fuels
680Bp	9/2/81	R. Almassy D. Eisenberg E. Westbrook C. Janson R.P. Phizackerley C. Cork E. Merritt (University of California-Los Angeles)	The Structure of Glutamine Synthetase
682Vp	9/3/81	J.W. Allen I. Lindau J. M. Lawrence Se-Jung Oh W. Ellis L. E. Cox (Xerox-PARC)	Resonant Photoemission Studies of Narrow Band Materials
684V	9/8/81	G.M. Rothberg (Stevens Institute of Technology)	Spin Polarized Photoelectron Studies of Magnetism in Solids (SPEXAFS)
686Mp	9/9/81	M.E. Leonowicz D. Vaughan P.M. Eisenberger J. M. Newsam G. B. Ansell (Exxon)	X-ray Structure Determinations from Crystals Less than 20 Microns in Diameter
690Bp	9/14/81	R.C. Elder E.A. Deutsch (University of Cincinnati)	Technetium Radiopharmaceutical Imaging Agents: EXAFS and Edge Studies

No.	Received	Experimenters	Title
698Bp	9/16/81	K.O. Hodgson S. Conradson B. Burgess W. Newton R. Holm (SSRL-Stanford University)	XAS of Bioinorganic Molybdenum and Related Systems: Nitrogenase and Xanthine Oxidase
700M	9/16/81	J.E. Penner-Hahn K.O. Hodgson I. Persson (Stanford University)	Structures of Mercury (II) Complexes in Solution
701Vp	10/17/81	I. Lindau M. Hecht (SSRL-Stanford University)	The Effect of Many-Electron and Solid State Phenomena on Partial Photoionization Cross Sections
702Mp	9/17/81	P.A. Montano W. Schulze T. Morrison (University of West Virginia)	EXAFS and XANES Studies of Matrix-Isolated Metal Clusters
706Mp	10/24/81	W.K. Warburton K. Ludwig L. Wilson J. Hoyt (SSRL-Stanford University)	Partial Structure Factor Determination in Binary Liquids by Anomalous X-ray Scattering
708Mp	10/29/81	S. C. Moss K.S. Liang C. Thompson (University of Houston)	Structural Studies of Ordering in Intercalates of Graphite and TiS_2
710B	10/2/81	B. Muhoberac B. Chance L. Powers D. Wharton P. Horowitz (University of Texas-San Antonio)	Structural Studies of the Catalytic Center(s) of Pseudomonas Cytochrome Oxidase
713Mp	10/16/81	D.E. Moncton R.S. Pindak (Bell Laboratories)	High Resolution Study of Liquid Crystal Thin Films
716Mp	2/25/82	P.S. Pershan J. Collett L.B. Sorensen E. Sirota (Harvard University)	High Resolution Study of Structural Phase Transitions in Freely-Suspended Liquid Crystal Films
717M	3/1/82	J.G. Gordon L. Blum (IBM Research Laboratory)	Study of EXAFS from Wet Electrode Surfaces
718M	3/1/82	R. Dalla-Betta M. Boudart (Stanford University)	Characterization by XAS of Burwell-Type Catalysts for CO-H_2 Reactions
719M	3/1/82	O. Shimomura T. Kawamura T. Fukamachi S. Wakoh (Nat. Inst. for Res in Inorganic Materials)	X-Ray Absorption Study of Pressure-Induced Electronic Transition in Cesium
720Mp	3/1/82	M. Sutton R.J. Birgeneau P. Horn D. Moncton (MIT)	Multilayer Adsorption on Graphite
721M	3/1/82	D. Sandstrom (Washington State University)	Study of Strong Electrolytes by X-Ray Spectroscopy at the Cl K-edge

No.	Received	Experimenters	Title
722M	3/1/82	T.I. Morrison G.K. Shenoy D.M. Gruen M. Pellin P.A. Montano (Argonne National Lab)	X-Ray Absorption Studies of Rare Gas Matrices
723B	3/1/82	I.C. Baianu H.S. Gutowsky R.T. Govindjee (University of Illinois)	X-Ray Diffraction Studies of Magnetically Oriented Photosystem II Particles and Thylakoids
724M	3/1/82	M.B. Stearns S.P. Vernon (Arizona State University)	Radial Displacement Surrounding Solutes in Fe, Ni and Cu
725M	3/1/82	M.B. Stearns S. Vernon (Arizona State University)	Bond-Lengths and Local Environment Studies Surrounding Mn, Rb Sr and Y Solutes in Ca F_2 and Pb F_2
726M	3/1/82	M.B. Stearns S.P. Vernon (Arizona State University)	Strain Induced Effects Surrounding Impurity Cations (X = Mn,Fe,Co,Ni,Zn) in the Rutile Systems $Mn_{1-x}X_xF_2$ and $Ni_{1-x}X_xF_2$
727Vp	3/3/82	R. Tatchyn E. Kallne I. Lindau R.Z. Bachrach (SSRL-Stanford University)	Optical Constants in the X-Ray Region Using Transmission Gratings
728Vp	3/3/82	R. Tatchyn E. Kallne P. Csonka I. Lindau (SSRL-Stanford University)	X-Ray Diffraction Properties of Transmission Gratings and Zone Plates
729V	3/5/82	C.R. Brundle D.J. Auerbach I. Lindau J. Behm (IBM Research Laboratory)	Photoemission Studies of Oxygen Adsorbed on W(100) and (110) Surfaces
730B	3/5/82	J. Wong T.E. King A.J. Yencha (General Electric)	EXAFS Studies of Respiratory Succinate Dehydrogenase
731B	3/8/82	B. Chance L. Powers Y. Ching B. Kincaid D. Bickar (University City Science Center)	Anomalous X-Ray Scattering Studies of Dense Cytochrome Oxidase
732B	3/8/82	L. Powers B. Chance A. Lehninger Y. Cheung (Bell Laboratories)	Calcium Edge and EXAFS Studies of Biological Molecules
733Vp	3/8/82	E. Solomon (Stanford University)	UPS Studies of the Coordination Chemistry of Metal Oxide and Chloride Surfaces
734M	3/9/82	M.R. Farrar P.L. Soni F. Khambatta (Raychem Corporation)	SAXS from Unfilled and Filled Polymer Resins

No.	Received	Experimenters	Title
735Mp	3/9/82	T. Kendelewicz I. Lindau J. Stohr (SSRL-Stanford University)	Surface EXAFS Studies of Solid-Solid Interface Formation Schottky Barriers
736Vp	3/15/82	V. Rehn R.A. Rosenberg A.K. Green P.R. Laroe P.J. Love (Michelson Laboratory)	MLSRP Research on Bulk and Surface EXAFS of Light Atoms
737Vp	3/15/82	V. Rehn R.A. Rosenberg A.K. Green P.R. Laroe P.J. Love G. Thornton I. Owen (Michelson Laboratory)	MLSRP Research in the Surface Chemistry of Electronic Materials
738Vp	3/15/82	V. Rehn R.A. Rosenberg A.K. Green P.R. Laroe P.J. Love (Michelson Laboratory)	MLSRP Research on Cryogenic Molecule Films
739M	3/16/82	P.M. Sanda S. Brennan G-C. Wang (Exxon)	Structural Studies of Tungsten (100) Using Grazing - Incidence X-Ray Scattering
740M	3/22/82	S.B. Qadri E.F. Skelton A.W. Webb (Naval Research Laboratory)	Structural Studies of Ternary Chalcopyrite Semiconductors at Elevated Pressures and Temperatures
741M	3/22/82	G.E. Brown G.A. Waychunas J. Tossell (Stanford University)	K-Edge and EXAFS Study of Na, K, and Ca in Amorphous and Crystalline Aluminosilicates
742Mp	3/29/82	P. Horn P Dimon (IBM Watson Research Center)	Multicritical Melting of Xenon on Graphite
743Mp	3/30/82	S. Brennan P. Eisenberger (National Bureau of Standards)	SEXAFS/Surface Bragg Scattering Studies of Structure and Dynamics
744Vp	4/1/82	B. Abeles (Exxon)	Photoelectron Spectroscopy of A-SiH$_x$ and of Heterojunctions of A-SiH$_x$ with Other Semiconductors
745M	4/6/82	I. Robinson G. Aeppli D. Moncton (Bell Laboratories)	Nitrogen Orientation on Graphite
746M	4/19/82	E.F. Skelton J.L. Feldman S.B. Qadri (Naval Research Laboratory)	Composition Studies of ThF$_4$ Thin Films
747M	4/30/82	J.C. Mikkelsen J.B. Boyce (Xerox PARC)	Study of Vegard's Law in Pseudobinary Solid Solutions

No.	Received	Experimenters	Title
748Bp	5/5/82	H.M. McConnell M. Seul P. Eisenberger (Stanford University)	X-ray Total External Reflection Studies on Phospholipid Monolayers
749M	5/18/82	I. Freund G. Brown (Bar-Ilan University)	Parametric Down Conversion of Synchrotron X-Radiation into the Extreme Ultra-Violet
750M	5/18/82	A.W. Webb E.F. Skelton S.B. Qadri J.F. Cannon (Naval Research Laboratory)	Compressibility and Thermal Expansion Under Pressure of Ni_3 Sn and Related Materials
751Mp	5/26/82	S.A. Wolf E.F. Skelton P.M. Chaikin C.Y. Huang (Naval Research Laboratory)	Low Temperature and High Pressure Structural Studies of Anisotropic and Organic Conductors and Superconductors
752M	6/7/82	J. Wong K.J. Rao (General Electric)	Bonding and Structure of Pb in Novel $PbO-PbCl_2$ Glasses Using Xanes and EXAFS
753M	6/10/82	J. Wong K.J. Rao (General Electric)	Structure and Bonding in Novel Ionic Sulphate Glasses
754Mp	6/13/82	R.B. Greegor F.W. Lytle R.C. Ewing R.F. Haaker (Boeing Company)	X-ray Spectroscopic Investigation of Metamict Minerals
755M	7/15/82	T.P. Russell (IBM Research Laboratory)	Phase Separation of Low Molecular Weight Polymer Mixtures
756V	7/30/82	R.D. Bringans R.Z. Bachrach (SSRL-Stanford University)	Hydrogen Interaction with the GaAs(111) Surface
757V	8/31/82	D.G. Stearns A.I. Bienenstock (Stanford University)	Time-Resolved Photoluminescence Decay in Hydrogenated Amorphous Silicon
758M	8/31/82	D. de-Fontaine J.P. Simon J.J. Hoyt R. Pro W. Warburton (University of California-Berkeley)	Three-Radiation Analysis of Spinodal Decomposition
759B	8/31/82	I.C. Baianu T. Nishida (University of Illinois)	Small-Angle X-ray Scattering of Lecithin-Cholesterol Acyltransferase
760M	8/31/82	M. Marcus (Bell Laboratories)	Impurity-Host Interaction in Metallic-Glass Forming Systems
761Bp	8/31/82	R.A. Scott S.P. Cramer H. Beinert (University of Illinois)	XAS Studies on the Active Sites of Cytochrome c Oxidase

No.	Received	Experimenters	Title
762Bp	8/31/82	R.A. Scott T.B. Rauchfuss H. Beinert K.O. Hodgson J.E. Penner-Hahn (University of Illinois)	Structural Aspects of Iron-Sulfur Clusters in Proteins and Models
764V	8/31/82	R.Z. Bachrach B.A. Huberman (Xerox PARC)	Study of Surface Phase Transitions and Surface Melting: Aluminum and Silicon
765M	10/2/82	P.A. Montano P.P. Vaishnava (West Virginia University)	EXAFS Study of Iron Sulfides and Ni-Mo During Coal Liquefaction
766M	9/2/82	R.A. Scott T.B. Rauchfuss T.D. Weatherill (University of Illinois)	Structure Determination by XAS. Some Intriguing Fe-S and Co-S Clusters
767V	9/1/82	B.B. Pate J.A. Kelber W.E. Spicer I. Lindau (Stanford University)	H+ Desorption by Valence Excitation of Diamond:Hydrogen
768M	9/2/82	J.F. Brazdil R.G. Teller R.K. Grasselli M. Mehicic M.R. Antonio D.R. Sandstrom (Standard Oil Company)	X-ray Absorption Study of Bismuth Molybdate Catalysts
769M	9/2/82	M. Tenhover M. Mehicic M.R. Antonio P. Boolchand D.R. Sandstrom (Standard Oil Company)	Structural Study of Ge-Sn-Se-S Glasses by X-ray Absorption Spectroscopy
770M	9/2/82	B. McQuillan J.V. Acrivos (GA Technology)	Studies of the Vanadium Site Symmetry in Various Oxides and Oxyanions
771V	9/3/82	L. Braicovich I. Abbati G. Rossi J. Nogami I. Lindau S. Nannarone U. Del-Pennino C. Carbone (Inst. Di Fisica Del Polit Di Milano)	Study of the Formation of Rare Earth Elemental Semiconductor (Ge,Si) Compounds and Interfaces
772V	9/3/82	L. Braicovich I. Abbati G. Rossi J.J. Yeh I. Lindau U. Del-Pennino S. Nannarone C. Calandra F. Manghi C. Carbone (Inst Di Fisica Del Polit Di Milano)	Solid State and Chemical Bonding Effects on the Cross Sections for Photoionization
773M	9/2/82	J.V. Acrivos B. McQuillan (San Jose State University)	X-ray Diffraction and Absorption Studies of Periodic Lattice Distortions

No.	Received	Experimenters	Title
774B	9/2/82	B.R. Stults F.W. Lytle R.B. Greegor S.M. Schuster (Monsanto Company)	X-ray Absorption Studies of Phosphoryl Transfer Reactions
775M	9/2/82	M. Mehicic J.F. Brazdil R.K. Grasselli M.R. Antonio D.R. Sandstrom (Standard Oil Company)	X-ray Absorption Spectroscopy Study of the Binary Molybdate Catalysts $A_xB_{2-x}(MoO_4)_3$
776M	9/2/82	K.O. Hodgson A.R. Siedle L. Kevan (SSRL-Stanford University)	Molecular Models for Metal-Oxide Surface Interactions
777M	9/2/82	R.A. Scott J.R. Shapley W.S. Uchiyama (University of Illinois)	XAS Studies of Supported Catalysts, Mo-Ir Clusters on Alumina
778V	9/7/82	L. Golub E. Kallne E. Spiller R. Bartlett (Harvard-Smithsonian Astrophysics Observatory)	X-ray Test of Multilayer Coated Optics
779Mp	9/7/82	G.S. Brown G.E. Ice B. Crasemann M.H. Chen G.B. Armen J. Levin (SSRL-Stanford University)	Gas-Phase Threshold Electron Spectrometry of Atomic Inner Shells
780M	9/14/82	B.M.L. Rao K.S. Liang L. Chiang R.B. Long S. Laderman A. Bienenstock (Exxon)	Study of Precipitate Nucleation and Molecular Association in Asphaltene Solutions
781B	9/15/82	K.O. Hodgson E.I. Solomon M.S. Co T.A. Smith J. Penner-Hahn (SSRL-Stanford University)	Polarized X-ray Absorption Spectroscopy on Oriented Hemocyanins
782M	9/15/82	M.H. Manghnani L.C. Ming D. Schiferl B.F. Shelton (University of Hawaii)	In Situ High Pressure-High Temperature X-ray Diffraction Studies for Investigation of Phase Transformations in Mantle Phases and the Equation of State of Gold: Application in Geochemistry and Geophysics
783Mp	9/15/82	D.G. Castner T.R. Hughes P.R. Watson W.L. Dimpfl (Chevron Research Company)	X-ray Absorption Studies of Platinum-Zeolite Catalysts
784B	9/20/82	S.P. Cramer (Exxon)	X-ray of Active Molybdenum Cofactor
785B	9/20/82	S.P. Cramer R. Hille R. Stewart V. Massey (Exxon)	Mo and As EXAFS of Substrate Complexes of Arsenite-Inhibited Xanthine Oxidase

No.	Received	Experimenters	Title
786Vp	9/29/82	D. C. Lorents T.G. Slanger G.K. Walters (SRI International)	Spectroscopy and Kinetics of Excited Gases
787B	9/29/82	C. Borso P. Thiyagarajan M. Johnson (Argonne National Laboratory)	Time Resolved Small Angle Scattering Study of Deoxygenated Sickled Hemoglobin
788M	10/1/82	K. Ludwig W. Warburton A. Bienenstock (Stanford University)	X-ray Study of the Structural Transition in Molten Se_xTe_{1-x}
789M	10/1/82	A. Fischer-Colbrie P. Fuoss M. Marcus A. Bienenstock (Stanford University)	X-ray Scattering Studies of Very Thin Disordered Layers
790B	10/4/82	D.E. Sayers E.C. Theil E.A. Stern P.M. Harrison (North Carolina State University)	X-ray Absorption Studies of the Protein-Iron Interface in Ferritin
791Mp	10/5/82	G.H. Via R. Madon J. Brown L. Murrell J. Horsley F. Lytle (Exxon)	X-ray Absorption Studies of Strong Metal Support Interactions
792M	10/6/82	C.R. Safinya K.S. Liang N.A. Clark D.H. Van-Winkle S. Laderman (Exxon)	High Resolution X-ray Studies of Freely Suspended Thin Strand Discotics
793M	10/11/82	K. D'Amico D.E. Moncton (Brookhaven National Laboratory)	X-ray Studies of Atomic Microclusters
794Mp	10/12/82	K.O. Hodgson E.I. Solomon J.E. Penner-Hahn T.A. Smith S. Cohen S. Doniach M.A. Berding (SSRL-Stanford University)	X-ray Absorption Edge Structure as a Probe of Electronic Structure
795M	10/18/82	R.M. Fleming D.E. Moncton (Bell Laboratories)	Charge-Density Waves in Linear Chain Compounds
796M	10/19/82	R.M. Suter J.A. Rayne (Carnegie-Mellon University)	Studies of Interfacial Reactions in Thin-Film Couples
797M	10/22/82	T.I. Morrison D.L. Price G.K. Shenoy S. Susman (Argonne National Laboratory)	P-Edge EXAFS Studies of P_xSe_{1-x} Glasses

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798Mp	1/5/83	C.Y. Huang S.B. Quadri E.F. Skelton S.A. Wolf P.M. Chaikin (Los Alamos National Laboratory)	Structural Transitions In C_8 and C_8-T_h-R_8 as a Function of Pressure and Temperature
799Mp	1/18/83	N.M. Ceglio A.M. Hawryluk H. Medecki W. Warburton (Lawrence Livermore National Laboratory)	Development of an X-Ray Microscope with Submicron Resolution
800B	1/31/83	C.E. Bugg S. Ealick F.L. Suddath W.J. Cook R.P. Phizackerley C.W. Cork E.A. Merritt (University of Alabama in Birmingham)	High-Resolution Diffraction Studies of Scorpion Neurotoxin
801Vp	2/4/83	J. Stohr E. Muetterties A. Johnson (Exxon)	Surface NEXAFS and EXAFS of Complex Molecules
802B	2/14/83	F.S. Mathews P.H. Bethge M. Shamala L. Lim R.P. Phizackerley C.W. Cork E.A. Merritt (Washington University Medical School)	Flavocytochrome b_2 Structure Analysis by Anomalous Scattering Using Synchrotron Radiation
803M	2/16/83	A.R. Kortan R.J. Birgeneau M.S. Dresselhaus S.G.J. Mochrie (MIT)	Melting of a Two Dimensional Stripe Domain System
804M	2/16/83	M. Boudart G. Bergeret G.Meitzner (Stanford University)	Anomalous X-Ray Scattering and X-Ray Absorption Study of Pt-Mo Bimetallic Clusters
805Bp	2/28/83	H.M. McConnell P. Eisenberger M. Seul (Stanford University)	Surface Diffraction By Antibodies Bound to Lipid Haptens
806Mp	3/1/83	R.C. Elder W.R. Heineman (University of Cincinnati)	XASEGS: X-Ray Absorption Spectroscopy of Electrochemically Generated Species, a New Technique
807M	3/2/83	P.W. Stephens P.A. Heiney B. Ovryn (State University of New York-Stony Brook)	Studies of Commensurate-Incommensurate Transitions in Physiadsorbed Monolayers
808M	3/2/83	W.T. Elam E.F. Skelton J.L. Feldman I.L. Singer K.S. Grabowski S.B. Qadri (Naval Research Laboratory)	Investigation of the Atomic Geometry of Ion-Implanted Ti in Iron and Steel Surfaces

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809B	3/9/83	D. Eisenberg L. Aha (University of California-Los Angeles)	X-Ray Diffraction of Eye Lens
810Vp	3/7/83	W. Eberhardt J. Stohr E.W. Plummer (Exxon)	Fragmentation of Organic Molecules Following Soft X-Ray Excitation
811M	3/7/83	J.M. Jaklevic F.S. Goulding E.E. Haller A.C. Thompson J.T. Walton (University of California-LBL)	Investigation of Semi-Conductor Radiation Detector Properties Using Synchrotron Radiation
812M	3/8/83	G.A. Waychunas G.E. Brown Jr. J.L. Pressesky (Stanford University)	High Temperature EXAFS Study of Fe and Ni in Silicate Crystals and Melts
813M	3/11/83	R.J. Birgeneau P.M. Horn D.E. Moncton M. Sutton (MIT)	Re-entrant Melting of Krypton in Two Dimensions
814Mp	3/14/83	R.D. Lorentz A.I. Bienenstock (Stanford University)	Structural Investigations of Amorphous Fe_xGe_{1-x} Alloys
815M	3/14/83	J.T. Koberstein T.P. Russell E. Merritt (Princeton University)	Annealing Induced Changes of Segmented Polyurethane Block Copolymers
818V	3/17/83	R.H. Stulen T.E. Felter S.J. Haney M.L. Knotek (Sandia National Laboratories)	Near Threshold Photon-Stimulated Desorption
819Mp	3/21/83	S.S.P. Parkin K. Lee J.V. Acrivos (I.B.M. Research Laboratory)	X-Ray Absorption Studies of Transition Metal Thin Film Structures
820M	3/21/83	S.S.P. Parkin J.V. Acrivos (I.B.M. Research Laboratory)	X-Ray Absorption Studies of Organic Linear Chain Conductors
821B	3/22/83	G.C. Dismukes S.P. Cramer (Princeton University)	X-Ray Absorption of a Photosynthetic Mn Protein
822V	4/19/83	G. Kaindl W.D. Brewer I. Lindau D.A. Shirley J.J. Barton C.C. Bahr S.W. Robey L.E. Klebanoff (Freie Universitat Berlin)	M-Edge Soft X-Ray Spectroscopy of Mixed-Valent Rare Earth Compounds
823V	4/19/83	M.-L. Shek I. Lindau W.E. Spicer (Stanford University)	Photoemission Studies of Chemisorption-Induced Changes in Substrate Valence Electronic Structure
824Mp	9/1/83	J. Wong G. Slack (General Electric)	Metal-Doped Boron Thermoelectric Materials

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825B	9/1/83	B. Chance C. Kumar J.S. Leigh, Jr. R. LoBrutto Z.R. Korszun S. Khalid L. Parkhurst (Univ. of Pennsylvania)	Low Temperature Photolysis/Recombination of Hemoproteins Under Conditions of Nuclear Tunneling
826B	9/1/83	B. Chance J. Davis C. Kumar Y. Zhou Z.R. Korszun S. Khalid L. Parkhurst B. Vallee H. Winick (Univ. of Pennsylvania)	Flow Apparatus Tests of Hem-protein Reactions at High Beam Intensities
827M	9/1/83	I.K. Robinson P.H. Fuoss J. Stark P.A. Bennett (Bell Laboratories)	X-ray Structure Determination of Si(111) 7x7
828M	9/1/83	F.G. Bridges J.B. Boyce (University of California-Santa Cruz)	The Off-Center Displacement of Ag^+ Ions in Alkali Halides
829Mp	9/1/83	F.W. Lytle R.B. Greegor D.R. Sandstrom (Boeing Co.)	Optical Luminescence Excited by X-ray Absorption
830Mp	9/1/83	F.W. Lytle R.B. Greegor (Boeing Co.)	Determination of Electronic and Structural Parameters in Fast Ion Transport Materials
831B	9/1/83	J.H. Freedman L. Powers J. Peisach (Albert Einstein College of Medicine)	The State of Accumulated Copper in Hepatoma Cells
832M	9/1/83	J.T. Hoggins P.N. Ross, Jr. M.L. Deviney (Ashland Chemical Co.)	Characterization of Bimetallic Electrocatalysts in Cathodes
833Mp	9/1/83	M. Boudart J.S. Arrieta (Stanford University)	In Situ Characterization of Hydroprocessing Catalysts by X-ray Absorption Spectroscopy
834M	9/1/83	M. Boudart M.A. McDonald (Stanford University)	In Situ Characterization of Iron Fischer-Tropsch Catalysts
835M	9/1/83	B. McQuillan (GA Technologies, Inc.)	Applications of Group Theory to X-ray Edge Spectra
836Bp	9/1/83	H. Huang T.Y. Teng X.F. Wang (Rice University)	Structural Dynamics of Photolyzed Hemoproteins by 100 s-Resolved EXAFS and Optical Absorption
837Mp	9/1/83	J.D. Litster S. Kumar J. Brock B.D. Larson (M.I.T.)	Structure of Micellar Liquid Crystals

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838B	9/1/83	J. Wong A.J. Yencha Q.W. Wang T.E. King (General Electric)	EXAFS and XANES Studies of Bovine Heart Type II Nadh Dehydrogenase
839Mp	9/1/83	L. Eyring S.H. Lin T. Groy A. Holladay (Arizona State University)	X-ray Diffraction from Specimens Undergoing Solid State Chemical Reactions
840Bp	9/1/83	M.P. Klein V. Yachandra A. McDermott R.D. Britt S. Un R. Guiles K. Sauer (University of California-LBL)	X-ray Spectroscopy of Manganese and Iron in Chloroplasts
841B	9/1/83	M.P. Klein V. Yachandra R.D. Britt S. Un R. Guiles J. Fee (University of California-LBL)	X-ray Spectroscopy of Manganese and Iron in Superoxide Dismutases
842V	9/1/83	R.S. Williams (University of California-Los Angeles)	Electronic Structure of Gold Intermetallic Compounds with Gallium and Indium
843V	9/1/83	M.H. Hecht F.J. Grunthaner P.J. Grunthaner P. Pianetta (Jet Propulsion Laboratory)	Large Depth-of-Field Photoemission Probe of Si Interfaces Using Jumbo
844Mp	9/6/83	G.K. Shenoy T.I. Morrison D.L. Price S. Susman (Argonne National Laboratory)	Structural Study of Silicon and Germanium Chalcogenide Glasses
845M	9/1/83	M. Boudart G. Zhang (Stanford University)	Characterization of Gold Clusters Generated by a New Photochemical Method
846Bp	9/6/83	S.G. Boxer A. Kuki R. Moog P. Santangelo L. Takiff (Stanford University)	Time Resolved Fluorescence Studies of Photosynthetic Reaction Centers and Models
847M	9/14/83	K.D. Keefer T.A. Michalske W.L. Smith D.P. Evans (Sandia National Laboratory)	Measurement of Transformation Zone Profiles in Phase Transformation Toughened Glass Ceramics
848Mp	9/14/83	P.M. Horn J. Morar (IBM T.J. Watson Research Center)	The Melting Transition of Krypton and Xenon on MgO
849Mp	9/19/83	A. Fontaine W.K. Warburton K. Ludwig, Jr. J. Hoyt L. Wilson (LURE)	Determination of F' in Semiconductors Using a Prism

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850B	9/19/83	E. Sinn K.O. Hodgson (University of Virginia)	Di-Iron and Modified Acid Phosphatases
851B	9/20/83	S. Doniach K.O. Hodgson R.H. Fairclough J.L. Ranck M.V. Katre R.M. Stroud (Stanford University)	Small Angle-Ray Scattering Studies of Bacteriorhodopsin in Purple Membrane
852B	9/20/83	S. Doniach K.O. Hodgson S.R. Hubbard C.B. Klee (Stanford University)	Anomalous Small Angle X-ray Scattering From Calcium Binding Proteins in Solution
853B	9/21/83	S. Doniach S. Hubbard R.H. Fairclough K.O. Hodgson R.M. Stroud (Stanford University)	Small Angle X-ray Diffraction Studies of the Acetylcholine Receptor
854B	9/21/83	S. Doniach K.O. Hodgson J.L. Ranck P.N.T. Unwin (Stanford University)	Monolayer X-ray Diffraction Studies of Purple Membrane Bacteriorhodopsin
855M	9/21/83	C.E. Williams W.K. Warburton (SSRL-LURE)	Structural Studies of Ion-Containing Polymers
856B	9/22/83	H.M. McConnell M. Seul (Stanford University)	Diffraction by Molecular Films on Solid Substrates
857Mp	9/23/83	F. Comin J.M. Phillips P.H. Citrin (Bell Laboratories)	Structure and Nucleation Mechanism of Transition Metal Silicide Using SEXAFS
858M	9/27/83	S.S. Laderman A. Bienenstock K.S. Liang J.D. Passaretti R.R. Chianelli (Stanford University)	EXAFS Studies of Noncrystalline RuS_2 and OsS_2
859B	10/4/83	T.G. Spiro L. Powers B.M. Hoffman (Princeton University)	EXAFS Studies of Fe, Mn Hybrid Hemoglobins
860Mp	10/4/83	M. Bloch S. Garoff P. Eisenberger (Brookhaven National Laboratory)	Structural Studies of Organic Thin Films on the Solid-Gas and Liquid-Gas Interface
861M	10/6/83	K.L. D'Amico D.E. Moncton (Brookhaven National Laboratory)	X-ray Studies of Rare Gases on a Graphite Single Crystal Surface

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862Bp	10/6/83	S.P. Cramer L.E. Mortenson R.N. Patel E.I. Stiefel C.L. Liu M.W.W. Adams L. Ljungdahl S. Ragsdale I. Yamamoto S.M. Hsu (Exxon)	EXAFS of 1-Carbon Substrate Metalloenzymes
863Vp	10/7/83	L. Braicovich I. Abbati I. Lindau W.E. Spicer J. Nogami C. Carbone J.J. Yeh S. Nannarone U. Del Pennino C. Calandra O. Bisi (Istituto di Fisica del Polit di Milano)	Study of the Formation of Rare Earth/Elements Semiconductor (Ge,Si) Interfaces and Compounds
864V	10/11/83	C.S. Fadley B. Sinkovic B.D. Hermsmeier E.L. Bullock M. Sagurton R.C. White Z. Hussain J. Lecante (University of Hawaii)	Spin-Polarized Core-Level Photoelectron Diffraction From Magnetically-Ordered Systems
865M	11/14/83	D.B. McWhan G. Aeppli D.E. Moncton J.P. Remeika (Bell Laboratories)	Time Resolved X-ray Scattering Study of Pressure Induced Ferroelectric Transition

XII SSRL EXPERIMENTERS AND PROPOSALS BY INSTITUTIONS

As of December 31, 1983 there were 455 experimenters from 102 institutions officially involved with active proposals at SSRL. In addition, approximately 100 others (graduate students, etc.) participated in work at the laboratory in collaboration with these scientists. Of these institutions 19 are from 11 different foreign countries. The 83 United States institutions include 49 universities, 22 private corporations and 12 government laboratories.

Universities: Albert Einstein College of Medicine, Arizona State University, Boston University, Brigham Young University, California State University-San Jose, Carnegie-Mellon University, Center for Astrophysics-Harvard, Duke Marine Biology Station, Georgia State University, Harvard Medical School, Harvard University, Johns Hopkins University, Massachusetts Institute of Technology, North Carolina State University, Northeastern University, Northwestern University, Princeton University, Rice University, Stanford University, State University of New York-Albany, State University of New York-Stony Brook, Stevens Institute of Technology, University of Alabama-Birmingham, University of California-Berkeley, University of California-Irvine, University of California-Los Angeles, University of California-San Francisco, University of California-Santa Cruz, University of Cincinnati, University of Colorado, University of Connecticut, University of Hawaii, University of Houston, University of Illinois, University of Maryland, University of Michigan, University of Nebraska, University of New Mexico, University of Oregon, University of Pennsylvania, University of Puerto Rico, University of Southern California, University of Texas-San Antonio, University of Virginia, University of Washington, University of Wisconsin, Washington State University, Washington University Medical School, West Virginia University.

Private Corporations: Ashland Chemical Co., Bell Laboratories, Boeing Company, Charles F. Kettering Research Laboratory, Chevron Research Company, Exxon Research and Engineering, GA Technology, General Electric R & D Center, Hewlett Packard Laboratories, IBM Research Laboratories-San Jose, IBM Research Laboratory-Watson Research Center, Jet Propulsion Laboratory, Lockheed Research Laboratory, 3M Central Research Laboratory, Monsanto, Raychem Corp., SRI International, Standard Oil Company, St. Jude's Hospital and Research Institute-Tennessee, University City Science Center, U.S. Steel, Xerox PARC.

Government Laboratories: Argonne National Laboratory, Brookhaven National Laboratory, Lawrence Livermore National Laboratory, Los Alamos Scientific Laboratory, Michelson Laboratories, National Bureau of Standards, National Institutes of Health, Naval Research Laboratory, Oak Ridge National Laboratory, Sandia Laboratories, Stanford Synchrotron Radiation Laboratory, University of California-Lawrence Berkeley Laboratory.

Foreign Institutions: Bar-Ilan University, Freie Universitat Berlin, Fritz Haber Institut der Max Planck, Hebrew University, Istituto di Fisica del Politecnico di Milano, Istituto di Fisica-Universita di Roma, Istituto di Fisica-Universita di Modena, L.U.R.E., National Institute for Research in Organic Materials, Saitama Institute Of Technology, Simon Fraser University, Universidad del Zulia, University of Library and Information Science, University of Lund, University of Manchester, University of Petroleum and Minerals, University of Sheffield, Yamanashi University, Zhejiang University.

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XIII PUBLICATIONS BASED ON WORK AT SSRL

The following is a list of publications submitted by SSRL Users which have appeared during this reporting period. The list represents 155 publications.

Allen, J. W., S. J. Oh (Xerox PARC), I. Lindau (SSRL-Stanford University), L. I. Johansson (Linkoping U.),
Resonant Enhancement Of Rare Earth Valence Band Photoemission At 3d Absorption Edges.
Submitted to Phys. Rev. B, Rapid Comm.(1983).

Allen, J. W., S. J. Oh (Xerox PARC), I. Lindau (SSRL-Stanford U.), L. I. Johansson (Linkoping U.),
Resonant Enhancement Of Rare Earth Valence Band Photoemission At 3d Absorption Edges.
Phys. Rev. B., to be published(1983).

Allen, J. W., S. J. Oh (Xerox PARC), M. B. Maple, M. S. Torikachvili (UC San Diego),
Large Fermi-Level Resonance In The Electron-Addition Spectrum Of CeRu(2) And CeIr(2).
Phys. Rev. B.(Rapid Commun.) 28,5347(1983).

Allen, J. W., (Xerox PARC),
The 4f Spectral Weight In Cerium Materials-Facts And Issues.
Less-Common Metals 93,183(1983).

Allen, J. W., S. J. Oh (Xerox PARC), I. Lindau (SSRL-Stanford University), L. I. Johansson (Linkoping U.),
Resonant Enhancement Of Rare Earth Valence Band Photoemission At 3d Absorption Edges.
Phs.Rev.B.,submitted(1983).

Antonio, Mark R., W. E. Cleland, B. A. Averill (U. of Michigan), B. K. Teo (Bell Labs),
Iron And Molybdenum Extended X-Ray Absorption Fine Structure Studies Of Double-Cubane Clusters Containing MoFe(3)S(4) Cores.
J. Amer. Chem. Soc.,105,3477(1983).

Babalola, I. A., (U. of Ibad an), W. G. Petro, W. E. Spicer (Stanford U.), T. Kendelewicz, I. Lindau (SSRL-Stanford U.),
The Ag-InP(110) Interface: Photoemission Studies Of Interfacial Reactions and Schottky Barrier Formation.
Phys. Rev. B., to be published(1983).

Barbee, T., (Stanford U.), J. H. Underwood (LBL & University of Calif-Berkeley), W. Warburton (SSRL-Stanford U.),
Determination Of The X-Ray Anomalous Dispersion Of Ti Made With A Ti/C Layered Synthetic Microstructure.
Z. fur Physik, to be published(1984).

Barton, J. J., C. C. Bahr, S. W. Robey, J. G. Tobin, L. E. Klebanoff, D. A. Shirley (University of Calif.-LBL), Z. Hussain (University of Petroleum And Minerals),
Direct Surface Structure Determination With Photoelectron Diffraction.
Phys. Rev. Lett. 51,#4,272-275(1983).

Barton, J. J., C. C. Bahr, S. W. Robey, L. E. Klebanoff, D. A. Shirley (LBL-U. of Calif.), Z. Hussain (U. of Petroleum & Minerals),
Angle-Resolved Photoemission Extended Fine Structure.
Conf. Proc. Advances In Soft X-Ray Sci. & Tech. Brookhaven(1983).

Bauer, R. S., P. Zurcher, H. W. Sang (Xerox PARC),
Inequality Of Semiconductor Heterojunction Conduction-Band Edge Discontinuity And Electron Affinity Difference.
Appl. Phys. Lett., Oct(1983).

Bauer, R. S., H. W. Sang (Xerox PARC),
On The Adjustability Of The 'Abrupt' Heterojunction Band Gap Discontinuity.
Surface Science 132(1983).

Bauer, R. S., (Xerox PARC),
Proc. 10th Annual Conf. On Physics & Chemistry Of Semiconductor Interfaces.
J. Vac. Sci. Tech. (1983).

Bauer, R. S., (Xerox PARC),
Role Of Metastable Surfaces In Determining MBE Heterojunction Structure: GaAs/Ge Interfaces.
J. Vac. Sci. Tech. B1,314(1983).

Bauer, R. S., (Xerox PARC),
Proc. Of The 2nd Trieste Semiconductor Symposium.
Surface Sci. 132(1983).

Bienenstock, A., H. Winick (SSRL-Stanford University),
Synchrotron Radiation Research-An Overview.
Physics Today,(June, 1983).

Blasie, J. K., J. M. Pachence, A. Tavormina, P. L. Dutton (U. of Pennsylvania), J. Stamatoff, P. Eisenberger (Bell Labs), G. Brown (SSRL),
The Location Of Redox Centers In The Profile Structure Of A Reconstituted Membrane Containing A Photosynthetic Reaction Center-Cytochrome c Complex By Resonance X-Ray Diffraction.
Biochim. et Biophys. Acta,723,350-357(1983).

Blasie, J. K., D. Pierce, D. Pascolini, A. Scarpa (U. of Pennsylvania), L. Herbette (U. of Connecticut), S. Fleischer (Vanderbilt, U.),
Static And Time-Resolved Structural Studies Of The Ca25 ATPase Of Isolated Sarcoplasmic Reticulum.
Ann NY Acad. Sci. 402,478-484(1983).

Boudart, Michel, J. B. Arrieta, R. A. Dalla Betta (Stanford U.),
Correlation Between Thiophene Hydrodesulfurization Activity & The Number Of First Sulfur Neighbors As Determined By EXAFS In Sulfided CoMo/-Al2O3.
J. Amer. Chem. Soc., in press(1983).

Boyce, J. B., R. M. Martin, J. W. Allen (Xerox PARC),
EXAFS And Near Edge Structures In Mixed Valent Sm(1-x)Y(x)S And The Energy Threshold Puzzle.
In EXAFS And Near Edge Structure, Vol.27 in Springer Series In Chem. Phys., edited by A. Bianconi, L. Incoccia, & S. Stipcich,Springer-Verlag,Berlin(1983).

Boyce, R., G. Brown, H. Hower, T. Pate, H. Winick (SSRL-Stanford University), E. Hussain (University of Petroleum & Minerals), E. Umbach (Tech. U. T. Munchen),
Undulator Studies At SSRL.
Nuc. Instr. & Meth., accepted for publication (1983).

Bringans, R. D., (SSRL-Stanford University), R. Z. Bachrach (Xerox PARC),
Hydrogen Chemisorption On The Polar Surfaces Of GaAs.
J. Vac. Science & Tech., A1, 676(1983).

Bringans, R. D., (SSRL), R. Z. Bachrach (Xerox PARC),
The Electronic Structure Of GaAs(100) And GaAs(111) From Angle Resolved Photoemission.
Ann of Israel Phys. Soc. 6,330(1983).

Brown, G., H. Winick (SSRL-Stanford University), K. Halbach (LBL & SSRL), J. Harris (SLAC),
Wiggler & Undulator Magnets-A Review.
Nucl. Instr. & Meth.,208,65-77(1983).

Brown, G., H. Winick (SSRL & Stanford University), P. Eisenberger (Exxon Research & Eng.),
The Optimization Of Undulators For Synchrotron Radiation.
Nucl. Instr. & Meth., 204,543-547(1983).

Bunker, Grant, (U. of Washington),
Application Of The Ratio Method Of EXAFS Analysis To Disordered Systems.
Nuc. Instr. & Meth. in Phys. Res. 207,437-444(1983).

Citrin, P. H., J. E. Rowe (Bell Laboratories),
Local Structure Of Adsorbates On Semiconductor Surfaces Using SEXAFS: A Brief Summary .
Surf. Sci. 132, 205-211(1983).

Citrin, P. H., J. E. Rowe (Bell Labs), P. Eisenberger (Exxon Res. & Eng.),
Direct Structural Study Of Cl on Si(111) And Ge(111) Surfaces: New Conclusions.
Phys. Rev. B. 28,2299-2301(1983).

Co, M. S., K. O. Hodgson, S. Doniach (Stanford University), W. A. Hendrickson (U.S. Naval Res. Lab.),
Multiple Scattering Effects In EXAFS Spectroscopy Of Oxygen-Bridged Iron Complexes. Possibility Of Angle Determination By EXAFS Analysis.
J. Amer. Chem. Soc. 105,1144-1150(1983).

Comin, F., J. E. Rowe, P.H. Citrin (Bell Laboratories),
Structure And Nucleation Mechanism Of Nickel Silicide On Si(111) Derived From Surface Extended X-Ray Absorption Fine Structure.
Phys. Rev. Lett. 26,2402-2405(1983).

Conradson, S., (Stanford University),
X-Ray Absorption Studies Of The Mo Site Of Nitrogenase.
Ph.D. Thesis at Stanford University, 1983.

Desjardins, S. R., K. W. Penfield, S. L. Cohen (MIT), R. L. Musselman (Principia College), E. I. Solomon (Stanford U.),
Detailed Absorption, Reflectance & UV Photoelectron Spectroscopic & Theoretical Studies Of The Charge Transfer Transitions Of CuCly: Correlation Of The Square Planar & The Tetrahedral Limits.
J. Am. Chem. Soc. 105, 4590(1983).

Eberhardt, W., J. Stohr (Exxon Research & Eng.), J. Feldhaus (Fritz Haber Institut), E. W. Plummer (U. of Pennsylvania), F. Sette (Brookhaven Nat. Lab.),
Correlation Between Electron Emission And Fragmentation Into Ions Following Soft X-Ray Excitation Of The N(2) Molecule.
Submitted to Phys. Rev. Lett.(1983).

P. Eisenberger, J.M. Newsam, M.E. Leonowicz, D.E. W. Vaughan (Exxon Research and Eng.),
Micro-Crystal X-Ray Diffraction. First Data From A 1000 Cubic Micron Zeolite Crystallite.
Submitted to Nature(1984).

Fine, J. M., J. J. Rusek, J. Eldridge, M. E. Kordesch, J. A. Mann, R. W. Hoffman (Case Western Reserve U.), D. R. Sandstrom (Washington State U.),
Comparison Of Thin Passive And Air-Oxidized Iron Films Using EXAFS And MES.
J. Vac. Sci. Tech. A-1(2), 1036-37(1983).

Goodin, David B., (U. of Calif-Berkeley),
The Local Structure Of Manganese In The Photosynthetic Apparatus And Superoxide Dismutase: An X-Ray Absorption Study.
Ph.D. Thesis, University of Calif--Berkeley(1983).

Greegor, R. B., F. W. Lytle (Boeing Company), D. R. Sandstrom (Washington State University), Joe Wong (General Electric Res. & Dev.), Peter Schultz (Corning Glass Works),
Investigation Of TiO(2)-SiO(2) Glasses By X-Ray Absorption Spectroscopy.
J. Non. Cryst. Sol. 55, 27-43(1983).

Guest, J. A., K. H. Jackson, R. N. Zare (Stanford University),
Determination Of Rotational Alignment Of N(2)+B(2)E+ And Co+B(2)E+ Following Photonization of N(2) And CO.
Phys. Rev. A.,28,04,2217-2228(1983).

Hahn, J. E., M. S. Co, K. O. Hodgson, D. J. Spira, E. I. Solomon (Stanford University),
Quantitative Cu(I) Determination Using X-Ray Absorption Edge Spectroscopy: Oxidation Of The Reduced Binuclear Copper In T2D Rhus Laccase.
Biochem. Biophys. Res. Comm. 112,737-745(1983).

Harris, J., P. Morton, J. Spencer (SLAC-Stanford University), H. Winick (SSRL-Stanford University),
Undulator Induced Resonances.
Conf. Proc. 12th Int. Conf. on High Energy Accel.,Fermi Lab.(Aug.,1983).

Hecht, M. H., (Stanford University), R. D. Bringans, I. Lindau (SSRL-Stanford University), R. Z. Bachrach (Xerox PARC),
Modeling A Soft X-Ray Wunder.
Nucl. Instr. & Methods, 208, 113(1983).

Huang, H. W., W. H. Liu, T. T. Teng, X. F. Wang (Rice University),
100 Microsecon-Resolved EXAFS Technique For Starting Protein Dynamics.
Rev. Sci. Instr. 54,(Nov.,1983).

Huffman, G.P., F. E. Huggins (U.S. Steel Corp.),
Analysis Of The Inorganic Constituents In Low-Rank Coals.
Amer Chem. Soc. Div. Fuel Chem. Preprint 28(4) 112-122(1983).

Huggins, F. E., G. P. Huffman (U. S. Steel Corp.), F. W. Lytle, R. B. Greegor (The Boeing Company),
An EXAFS Investigation Of Calcium In Coal.
Proc.Int. Conf. on Coal Science, Pittsburgh 679-82(Aug.,1983).

Hughes, E. B., H. D. Zeman, L. E. Campbell, R. Hofstadter, U. Meyer-Berkhout, J. N. Otis, J. Rolfe, J. P. Stone, S. Wilson (Stanford University), E. Rubenstein, D. C. Harrison, R. S. Kernoff (Stanford U. School of Medicine), A. C. Thompson (LBL, U. of Calif.), G. S. Brown (SSRL, Stanford U.),
The Application Of Synchrotron Radiation To Non-Invasive Angiography.
Nucl. Instr. & Meth. in Phys. Research 208:665(Apr.,1983).

Janson, C.A., R. J. Almassy, E. M. Westbrook, D. Eisenberg (UCLA),
Isolation And Crystallization Of Unadenylylated Glutamine Synthetase From S. Typhimurium.
Arch. Biochem. & Biophys. in press(1984)

Kaindl, G., (LBL-U.of Calif.), W. D. Brewer (SSRL-Stanford U.), G. Kalkowski (Frei U. Berlin), F. Holtzberg (IBM Watson Res. Ctr.),
M-Edge X-Ray Absorption Spectroscopy: A New Tool For Dilute Mixed Valent Materials.
Phys. Rev. Lett., in print(1983).

Kaindl, G., (Frei U. Berlin & LBL), G. Kalkowski, W. D. Brewer, B. Perscheid (Freie U. Berlin), F. Holtzberg (IBM Watson Res. Ctr.),
M-Edge X-Ray Absorption Spectroscopy Of 4f Instabilities In Rare-Earth Systems.
Submitted to Appl Physics, (1983).

Kendelewicz, T., (SSRL & Polish Acad. of Science), W. G. Petro, J. A. Silberman, W. E. Spicer (Stanford University), I. A. Babalola (University of Ibadan Lindau (SSRL & Stanford University),
Photoemission Studies Of [illegible] (110) Interface.
Phys. Rev. B, 27, 06,3366(1983).

Kendelewicz, T., (SSRL & Polish Acad. of Science-Warsaw), G. Rossi, W. G. Petro, W. E. Spicer (Stanford University), I. Lindau (SSRL & Stanford University), I. A. Babalola (University of Ibadan),
Similarities In Chemical Intermixing At The Cu/InP & Cu/Si Interfaces.
J. Vac. Sci. & Tech., to be published (1983).

Kendelewicz, T., (Polish Acad. of Sci. & SSRL), W. G. Petro, M. D. Williams, W. E. Spicer (Stanford U.), S. H. Pan (Nankai U.), I. Lindau (SSRL-Stanford U.),
Fermi Energy Pinning Behavioir And Chemical Reactivity Of The Pd/GaAs(110) Interface.
Appl. Phys. Lett. to be published(1983).

Kendelewicz, T., I. Lindau (SSRL-Stanford U.), W. G. Petro, W. E. Spicer (Stanford U.),
The Interaction Of Pd With The InP(110) Surface.
J. Vac. Sci. Tech., to be published(1983).

Kendelewicz, T., I. Lindau (SSRL-Stanford U.), W. G. Petro, W. E. Spicer (Stanford U.),
Evidence Of Palladium Phosphide Formation At The Pd/InP(110) Interface.
Phys. Rev. B.,28,3618(1983).

Kobrin, P. H., S. Southworth, C. M. Truesdale, D. W. Lindle, U. Becker, D. A. Shirley (LBL & University of California-Berkeley),
Threshold Measurements Of The K-Shell Photoelectron Satellites In Ne And Ar.
Submitted to Physical Review A (1983).

Kobrin, P.H., P. A. Heimann, D.W. Lindle, C. M. Truesdale, T. A. Ferrett, D. A. Shirley (University of Calif.-LBL), H. G. Kerkhoff, U. Becker (LBL & Tech. U. of Berlin),
Photoelectron Measurements Of The Mercury 4f, 5p, and 5d Subshells.
Phys. Rev. A 27,06,3031-3039(1983).

Kobrin, P. H., R. A. Rosenberg, Becker U., S. Southworth, C. M.; Truesdale, D. W. Lindle, G. Thornton, M. G. White, E. D. Poliakoff, D. A. Shirley (LBL & University of California-Berkeley),
Resonance Photoelectron Spectroscopy Of 5p-Hole States In Atomic Barium.
Submitted to Journal of Physics B (1983).

Kordesch, M. E., R. W. Hoffman (Case Western Reserve U.),
Electrochemical Cells For In Situ EXAFS.
Submitted to Nuc. Instr. & Methods(1983).

Kordesch, M. E., R. W. Hoffman (Case Western Reserve U.),
Electron Yield EXAFS Using A Gas-Flow Electron Detector.
Submitted to Phys. Rev. B(1983).

Kortright, J., (Stanford U.), A. Bienenstock (SSRL),
Structural Studies Of Amorphous Mo-Ge Alloys Through The Semiconductor-Metal Transition.
J. Non-Cryst. Sol. to be published(1983).

Kortright, J., (Stanford University), W. Warburton, A. Bienenstock (Stanford University-SSRL),
Anomalous X-Ray Scattering And Its Relationship To EXAFS.
EXAFS And Near Edge Structure, ed. A. Bianconi, L. Incoccia And S. Stipcich, Springer-Verlag (1983).

Kortright, J., (Stanford University), A. Bienenstock (SSRL),
Structural Study Of Metallic Amorphous Mo-Ge Alloys.
J. Non-Cryst. Sol. to be published(1983).

Lederman, Stephen, (Stanford University),
Structural Studies Of Amorphous Semiconductors Containing Transition Metals.
Ph.D. Thesis, Stanford University (1983).

Lin, W. H., X. F. Wang, T. T. Tang, H. W. Huang (Rice University),
Micro Computer Controlled System Used In Time Resolved EXAFS Technique.
Rev. Sci. Instr. 54, (Dec., 1983).

Lindau, I., T. Kendelewicz (SSRL-Stanford U.), W. E. Spicer, W. G. Petro (Stanford U.),
Electronic & Structural Properties Of Thin Metal Overlayers On III-V Compounds.
Proc. of 9th Int. Vac. Congress & 5th Int. Conf. on Solid Surfaces, ed. by J.L. de Segovia, Assoc. Espanola del Vacio of sus Applic, Madrid,146-157(1983).

Lindau, I., (SSRL & Stanford University), M. H. Hecht (Jet Propulsion Laboratory),
Photoionization Processes Near The 4d Threshold In Ba Compounds

Annals Israel Physical Soc. 6,219(1983).

Lindle, D. W., T. A. Ferrett, U. Becker, P. H. Kobrin, C. M. Truesdale, H. G. Kerkhoff, D. A. Shirley (LBL & University of California-Berkeley),
Photoionization Of Helium Above The He+(n=2) Threshold: Autoionization And Final-State Symmetry.
Submitted to Physical Review A (1983).

Loubriel, G., M. L. Knotek, R. H. Stulen (Sandia National Labs), B. E. Koel, C. C. Parks (Univ. of Calif.-LBL),
Photon And Electron Stimulated Desorption From Rare Earth Oxides.
J. Of Vac. Sci. & Tech., A-1(2)1145-1148(1983).

Loubriel, G. M., (Sandia National Labs), C. C. Parks (University of Calif.-LBL),
Photon-Stimulated Desorption From Rare Earth Oxides.
Less Common Metals,93,213-218(1983).

Lytle, F. W., R. B. Greegor (Boeing Company), D. R. Sandstrom, E. C. Marques (Washington State U.), J. Wong, C.L. Spiro (General Electric), G. P. Huffman, F. E. Huggin (U.S. Steel Corp.),
Measurement Of Soft X-Ray Absorption Spectra With A Fluorescent Ion Chamber Detector.
Submitted to Nucl. Instr. & Meth.(1983).

Marques, E. C., (Washington State University),
Thermal Motion Of Surface Atoms In Silica Supported Platinum And Iridium Catalyst Clusters: An EXAFS Spectroscopy Study.
Ph.D. Thesis, Washington State University(1983).

Ming, L. C., M. H. Manghnani, J. Balogh (University of Hawaii), S. B. Qadri, E. F. Skelton (Naval Research Laboratory), J. C. Jamieson (University of Chicago),
Gold As A Reliable Internal Pressure Calibrant At High Temperature.
J. Appl. Phys., 54,4390-4397(1983).

Ming, Li Chung, M. H. Manghnani, J. Balogh (U. of Hawaii), S. B. Qadri, E. F. Skelton, A. W. Webb (Naval Research Lab.), J. C. Jamieson (U. of Chicago),
Static P-T-V Measurments On MgO: Comparison With Shock Wave Data.
Proc. Amer. Phys. Soc. Topical Conf. on Shock Waves In Condensed Matter(1983).

Mo, D., (Zhongshan U.), S. H. Pan (Nankai U.), W. G. Petro, P. Mahowald, K. K. Chin, W. E. Spicer (Stanford U.), I. Lindau (SSRL-Stanford U.),
Electronic Structure Evolution Of Au Deposited On GaAs(110).
Thin Solid Films, to be published(1983).

Nelson, Jeffrey G., W. J. Gignac, R. Stanley Williams (UCLA), S. W. Roby, J. G. Tobin, D. A. Shirley (LBL & University of California-Berkeley),
Angle-Resolved Photoelectron Spectroscopy Investigation Of Intrinsic Surface States On The Ge(001)-(2x1) Reconstructed Surface.
Phys. Rev. B. 27, 3924-3926(1983).

Nelson, Jeffrey. G., William J. Gignac, R. Stanley Williams (UCLA), S. W. Robey, D. A. Shirley, J. G. Tobin (LBL-U.C. Berkeley),
Mapping Bulk Ge Electronic Energy Bands Along Delta Using ARPES Spectra Of The (001) 2x1 Surface.
Surf. Sci. 131,290-298(1983).

Nielsen, M., J. Kjaer, J. Bohr (Riso Nat. Lab.), J. P. McTague (Brookhaven Nat. Lab.),
X-Ray Neutron Diffraction Measurements On Physisorbed Films On Graphite.
Journ. Elec. Spec. Rel. Phen. 30,111-118(1983).

Nielsen, M., J. Bohr, K. Kjaer, J. Als-Nielsen (Riso Nat. Lab.), J. P. McTague (Brookhaven Nat. Lab.),
Synchrotron X-Ray Diffraction Applied To The Study Of Physisorbed Monolayers.
Nucl. Instr. Meth. 208,549-554(1983).

Oh, S. J., J. W. Allen (Xerox PARC), I. Lindau (SSRL-Stanford U.), M. Campagna (Inst. Julich GmbH),
Soft X-Ray Resonant Photoemission Study Of Mixed-Valent TmSe.
Phys. Rev. B. to be published(1983).

Olson, C. G., D. W. Lynch, D. M. Wieliczka, F. S. Khumalo (Iowa State U.), R. J. Bartlett (Los Alamos Nat. Lab.),
Thermomodulated EXAFS Spectra Above The K-Edge In Cu and Fe.
J. Phys. C. :Solid State Phys. 16,3813-3823(1983).

Otis, J. N., H. D. Zeman, E. B. Hughes, L. C. Finman, R. Hofstadter, A. Hudson, J. Rolfe (Stanford University), E. Rubenstein, D. C. Harrison, S. Kernhoff (Stanford U. School of Medicine), A. C. Thompson (U. of Calif-LBL), G. S. Brown (SSRL-Stanford University),
Evaluation of Synchrotron X-Rays For Digital Subtraction Angiography.
Proc. of IEEE 1983 Nucl. Sci. Symposium, Oct.1983, San Francisco.

Parente, Fernando, (U. de Lisboa),
Inelastic X-Ray Scattering Cross Sections Of Ne.
J. Phys. B. At Mol. Phys.,16,3487-3501(1983).

Parkin, S.S.P., (IBM Research Lab.), J. V. Acrivos (San Jose State U.),
XANES In (TmTSeF) (2) ReOx: Polarization Dependence Of The Se K-edge.
J. de Physique, to be published(1983).

Parks, C. C., (LBL & University of Calif-Berkeley),
The Auger Decay Mechanism In Photon-Stimulated Desorption Of Ions From Surfaces.
Ph.D. Thesis, University of California-Berkeley(1983).

Parks, C. C., D. A. Shirley (LBL & University of Calif.-Berkeley), G. Loubriel (Sandia National Lab.),
Beam Exposure Dependence And Mechanisms Of Photon-Stimulated Desorption From Alkali Fluorides.
Submitted to Phys. Rev. B(1983).

Parks, C.C., D. A. Shirley (LBL-UC Berkeley), E. Hussain (U. of Petroleum & Minerals), M. L. Knotek, G. Loubriel (Sandia Lab.), R. A. Rosenberg (Michelson Lab),
The Auger Decay Mechanism In Photon-Stimulated Desorption From Solium Fluoride.
Phys. Rev.B,28,88(1983).

Pate, B. B., J. A. Silberman, Rossi. G., W. E. Spicer (Stanford U.), M. Oshima (Nippon U.), I. Lindau (SSRL-Stanford U.),
Carbon 1s Studies Of Diamond(111) Surface Shifts, Hydrogenation, And Electron Escape Lengths.
J. Vac. Sci.Tech. to be published(1983).

Petro, W. G., W. E. Spicer (Stanford U.), I. A. Babalola (U. of Ibadan), T. Kendelewicz, I. Lindau (SSRL-Stanford U.),
Unique Surface Reactions: Noble Metals On InP(110).
Submitted to Phys. Rev. Lett.(1983).

Petro, W. G., W. E. Spicer (Stanford U.), T. Kendelewicz, I. Lindau (SSRL-Stanford U.), I. A. Babalola (U. of Ibadan),
Noble Metal Interactions With The InP(110) Surface.
J. Vac. Sci. Tech., in press(1983).

Phizackerley, R. P., Z. U. Rek (Stanford University-SSRL), G. B. Stephenson, S. D. Conradson, K. O. Hodgson (Stanford University), T. Matsushita (Nat. Lab. for High Energy Physics), H. Oyanagi (Elect. Tech. Lab.),
An Energy-Dispersive Spectrometer For The Rapid Measurement Of X-Ray Absorption Spectra Using Synchrotron Radiation.
J. Appl. Chryst. 16,220-232(1983).

Qadri, S. B., E. F. Skelton, A. W. Webb.
High Pressure Energy Dispersive X-Ray Diffraction Studies Of Ge Using Synchrotron Radiation.
J. Appl. Phys. 54,3609-3611(1983).

Qadri, Syed B., Yan Yin (SSRL),
Polarization Calculation Using Integral Representation Of Bessel Functions Of Fractional Orders.
Proc. 3rd Nat. Conf. On Syn. Rad. Instru., BNL(Sept.,1583).

Rao, K. J., J. Wong (General Electric), M. J. Weber (Lawrence Livermore Nat. Lab.),
Bonding & Structure Of Nd(3+) In BeF(2) Glass By EXAFS & XANES Spectroscopy.
J. Chem. Phys., 78,6228(1983).

Rosenberg, R. A., P. R. LaRoe, V. Rehn (Michelson Lab), J. Stohr, R. Jaeger (Exxon Res. & Eng.), C. C. Parks (LBL-UC Berkeley),
K-Shell Excitation Of D20 And H20 Ice: Photoion And Photoelectron Yields.
Phys. Rev. B. 28, 3026(1983).

Rosenberg, R. A., P. R. LaRoe, V. Rehn (Michelson Lab), G. M. Loubriel (Sandia Lab.), G. Thornton (U. of Manchester),
Soft X-Ray Photoelectron Yield Spectrom Of InP(110) From 65 to 195 eV.
Phys. Rev. B. to be published (1983).

Rosenberg, R. A., P. S. Love, P. R. LaRoe, A. K. Green, V. Rehn (Michelson Lab.),
Photolysis Of Iron Carbonyl Using Synchrotron Radiation.
J. Am. Vac. Soc. to be published (1983).

Rosenberg, R. A., V. Rehn, A. K. Green, Pr. R. LaRoe (Michelson Labs.), C. C. Parks (LBL-UC Berkeley),
Electron Correlation & Hole Localization In Photon Stimulated Ion Desorption From Condensed N2,CO,& C2N2.
Phys. Rev. Lett. 51,915(1983).
(16101)

Rossi, G., J. Nogami, J. J. Yeh, I. Lindau (Stanford University),
Chemical Reaction At The Annealed Si/Yb Interface .
J. Vac. Sci. & Tech., B1,530-532(1983).

Rossi, G.., J. Nogami (Stanford University), I. Lindau (SSRL & Stanford University), L. Braicovich, I. Abbati (Ist. di Fisica del Polit. di Milano), U. del-Pennino (Ist. di Fisica del Universite di Modena), S. Nannarone (Universita di Roma),
First Spectroscopic Investigation Of The Yb/Si Interface At Room Temperature.
J. Vac. Sci. Tech., A1,781-84(1983).

Rossi, G.., (Stanford University), R. Jaeger, J. Stohr (Exxon Res. & Eng.), T. Kendelewicz, I. Lindau (Stanford University),
L-edge X-Ray Absorption Resonances In Palladium Silicides And Palladium Metal.
Phys. Rev. B, 27,5154(1983).

Rossi, G., (Stanford U.), I. Lindau (SSRL-Stanford U.),
Compound Formation & Bonding Configuration At The Si-Cu Interface.
Phys. Rev. B.28,3597(1983).

Rossi, G.., (Stanford University), I. Lindau (SSRL & Stanford University), L. Braicovich, I. Abbati (Ist. di Fisica del Pol. Milano),
Cooper Minimum Effects In The Photoionization Cross Sections Of 4d & 5d Electrons In Solid Compounds.
Phys. Rev. B, 28,3031(1983).

Rubenstein, E.., (Stanford University School of Medicine),
Medical Imaging With Synchrotron Radiation
Nuc. Instru. & Meth., to be published(1984).

Rubenstein, E.., (Stanford U. School of Medicine),
Medical Applications Of Synchrotron Radiation.
Conf. Proc. SSRL New Rings Workshop, July,1983.

Rubenstein, E.., (Stanford University),
Applications Of Synchrotron Radiation To Medical Imaging.
Nuc. Instr. & Meth. in Phys. Research, in press(1983).

Sandstrom, D. R.., E. C. Marques (Washington State University), F. W. Lytle, R. B. Greegor (Boeing Company),
Thermal Disorder In Pt and Ir Metal: Comparison of Model And Experimental Extended X-Ray Absorption Fine Structure.
Submitted to Phys. Rev. B15(1983).

Sayers, Dale E.., E. C. Theil, F. J. Rennick (North Carolina State U.),
A Distinct Environment For Iron III In The Complex With Horse Spleen Apoferritin Observed By X-Ray Absorption Spectroscopy.
J. Bio. Chem. 258,14876-14079(1983).

Seul, M.., H. M. McConnell (Stanford University), P. Eisenberger (Exxon Res. & Eng.),
X-Ray Diffraction By Phospholipid Monolayers On Single Crystal Silicon Substrates.
Nat. Acad. Sci. 80,5795-97(1983).

Shek, M. L.., P. M. Stefan, W. E. Spicer (Stanford University), I. Lindau (SSRL & Stanford University),
Electronic Structure Of Different Pt-Cu Surfaces.
Phys. Rev. B, 27,7288(1983).

Shek, M. L.., P. M. Stefan, W. E. Spicer (Stanford University), I. Lindau (SSRL & Stanford University),
CO Chemisorption On PtCu Surfaces: II (1x1)-CO/Pt(0.98)Cu(0.02)(110).
Surface Sci.,135,(1983).

Shek, M. L.., P. M. Stefan, W. E. Spicer (Stanford U.), I. Lindau (SSRL-Stanford U.),
CO Chemisorption On Cu Adlayers On Pt(111).
Phys. Rev. B.27,7301(1983).

Shek, M. L.., P. M. Stefan, W. E. Spicer (Stanford University), I. Lindau (SSRL & Stanford University),
A Photoemission Study Of The Adsorption Of Cu On Pt (111).
Phys. Rev. B.., 27,7277(1983).

Shek, M. L.., P. M. Stefan, W. E. Spicer (Stanford University), I. Lindau (SSRL & Stanford University),
CO Chemisorption On PtCu Surfaces: III. CO On PtCu(111).
Surface Sci.,135,(1983).

Shek, M. L., P. M. Stefan, W. E. Spicer (Stanford University), I. Lindau (Stanford University),
CO Chemisorption On PtCu Surfaces: I. CO On (1x3) Pt(0.98)Cu(0.02)(110).
Surface Sci.,135(1983).

Sheriff, S., W. A. Hendrickson, J. L. Smith (NRL),
Structure Of The Active Center Of Hemerythrins.
Life Chem. Reports,S1,305-308(1983).

Shirley, D. A., P. H. Kobrin, C. M. Truesdale, D. W. Lindle, T. A. Ferrett, P. A. Heimann, S. H. Southworth (LBL-U. of Calif.), U. Becker, H. G. Kerkhoff (Tech. U. Berlin & LBL),
Gas-Phase Photoemission With Soft X-Rays: Cross Sections And Angular Distributions.
Conf. Proc. Advances In Soft X-Ray Sci. & Tech.,Brookhaven(1983).

Silberman, J. A., W. E. Spicer (Stanford U.), D. Laser (Ministry of Defense-Israel), I. Lindau (SSRL-Stanford U.),
Initial Stages Of Oxide Formation On HgCdTe Exposed To Activated Oxygen.
J. Vac. Sci. Tech. to be published(1983).

Skelton, E. F., Webb. A. W., S. B. Qadri, S. A. Wolf, R. C. Lacoe, J. L. Feldman, W. T. Elam, E. R. Carpenter Jr., D. J. Nagel (NRL),
Energy-Dispersive X-Ray Diffraction With Synchrotron Radiation At Cryogenic Temperatures.
Submitted to Rev. Sci. Instru. (1983).

Skelton, E. F., (NRL),
High Pressure Research With Synchrotron Radiation.
Submitted to Physics Today(1983).

Skelton, E. F., A. W. Webb, D. J. Nagel, S. A. Wolf, I. Singer, S. B. Qadri (NRL),
Structural Investigations Of Solid Lubricants At Elevated Pressures And Temperatures Using Synchrotron Radiation:
Submitted to Tribology(1983).

Skelton, E. F., S. B. Qadri, A. W. Webb (Naval Research Laboratory), R. G. Ingalls, J. M. Tranquada (University of Washington),
Pressure Induced Disproportionation In CuBr.
Phys. Lett. 94A,441-443(1983).

Skelton, E. F., S. B. Qadri, A. W. Webb, C. W. Lee, J. P. Kirkland (Naval Research Laboratory);
An Improved System For Energy Dispersive X-Ray Diffraction With Synchrotron Radiation.
Rev. Sci. Inst., 54,403-409(1983).

Skelton, E. F., A. W. Webb, W. T. Elam, S. A. Wolf, S. B. Qadri (Naval Research Laboratory), C. Y. Huang (Los Alamos National Laboratory), K. A. Jr. Gschneidner (Iowa State University),
Structural Studies At Elevated Pressure And Reduced Temperature Using Synchrotron Radiation.
Conf proc. IXth Int. Assoc. for the Advancement of High Pressure Science & Tech. Conf., Albany, NY (1983).

Southworth, S., C. M. Truesdale, P. H. Kobrin, D. W. Lindle, D. A. Shirley (U. of Calif. and LBL), U. Becker (U. Calif. & LBL, Technische U. Berlin), S. Owaki (U. Calif. & LBL, Osaka University),
Electron Spectroscopy Study Of Inner-Shell Photoexcitation & Ionization Of Xe.
Phys. Rev. A 28,01,261-279(1983).

Spicer, W. E., J. A. Silberman, P. Morgen (Stanford University), I. Lindau (SSSRL & Stanford University), J. A. Wilson (Santa Barbara Research Center), An-Ban Chen (Auburn University), A. Sher (SRI International),
Unusual Behavior Of Hg(1-x)Cd(x)Te And Its Explanation.
Physica B, to be published (1983).

Spira, D. J., A. G. Porras, E. I. Solomon, J. E. Hahn, Co. M. S., K. O. Hodgson (Stanford U.),
X-Ray Absorption Studies Of Laccase & Ceruloplasmin.
Inorg. Chem. Acta 79,131-132(1983).

Spira, D. J., M. S. Co, E. I. Solomon, K. O. Hodgson (Stanford U.),
EXAFS Investigation Of The Binuclear Cupric Site In Met T2D Rhus Laccase And Its Azide Bound Derivative.
Biochem. Biophys. Res. Comm. 112,746-753(1983).

Spiro, T. G., G. L. Woolery, J. M. Brown (Princeton University), L. Powers (Bell Labs), M. E. Winkler, E. I. Solomon (Stanford University),
EXAFS Studies Of The Binuclear Copper Site Of Oxy-,Deoxy- And Met-Aquo,-Fluoro-,and -Azido-Hemocyanin From Arthropods And Molluscs..
In Copper Coord.Chem.:Biochem. & Inorg. Perspectives, eds. K.D. Karlin & J. Zubieta, Adenine Press, NY(1983).

Spiro, C. L., J. Wong, D. H. Maylotte, S. Lamson (General Electric), F. W. Lytle, R. B. Greegor (Boeing Company),
Direct Determination Of Sulfur Species In Coal.
Submitted to Nature(1983).

Stern, E. A., C. E. Bouldin (University of Washington), B. vonRoedern (Harvard U.), J. Azoulay (Tel Aviv U.),
Incipient Amorphous-To-Crystaline Transition In Ge.
Phys. Rev. B. 27,6557-6560(1983).

Stohr, J., (Exxon Res. & Eng.), R. Jaeger (Hewlett Packard), G. Rossi (Stanford U.), T. Kendelewicz (Polish Acad. of Sci. & SSRL), I. Lindau (SSRL-Stanford U.),
Structure Of The Ag On Si(111) 7x7 Interface By Means of Surface EXAFS.
Surf. Sci. to be published(1983).

Tatchyn, Roman, I. Lindau (SSRL-Stanford U.),
Transverse Undulator Spectra And Polarization Profiles.
Nucl. Inst. & Meth., to be published(1983).

Teo, B. K., (Bell Labs), M. R. Antonio, R. H. Tieckelmann, H. C. Silvis, B. A. Averill (Michigan State U.),
New EXAFS Models For The Iron Sites Of The Iron Molybdenum Cofactor Of Nitrogenase: The ((p-Ch(3)C(6)H(4)S)(2)FeS(2)FeS(2)MoS(2))3 Trianion And The ((C(6)H(5)O)(2)FES(2)MOS(2))(2) Dianion.
J. Amer. Chem. Soc.,104,6126(1983).

Thompson, A. C., J. Llacer (U. of Calif-LBL), L. C. Finman, E. B. Hughes, J. N. Otis, S. Wilson, H. D. Zeman (Stanford University),
Computed Tomography Using Synchrotron Radiation .
Nucl. Instru. & Meth., to be published(1984).

Tobin, J. G., S. W. Robey, L. E. Klebanoff, D. A. Shirley (LBL & University of California-Berkeley),
Ag/Cu(001): Observation Of The Development Of The Electronic Structure In Metal Overlayers From Two-To Three-Dimensionality.
Submitted to Physical Review Letters (1983).

Tobin, J. G., (LBL-UC. Berkeley),
Dimensionality & Its Effects Upon The Valence Electronic Structure Of Ordered Metallic Systems.
PhD. Thesis University of California Berkeley(1983).

Tranquada, John M., (U. of Washington),
X-Ray Absorption Studies Of Solids At High Pressure.
PhD Thesis, The University of Washington (1983).

Truesdale, C. M., P. H. Kobrin, D. W. Lindle, H. G. Kerkhoff, D. A. Shirley (University of Calif.-LBL), S. H. Southworth (University of Calif.-LBL & Nat. Bureau of Standards), U. Becker (U. of Calif.-LBL & Tech.. Univ. Berlin),
Shape Resonance Phenomena In CO Following K-Shell Photoexcitation.
Phys Rev Lett 50,017, 1265-1268(1983).

Truesdale, C. M., D. W. Lindle,
P. H. Kobrin, P. A. Heimann, T. A.
Ferrett, D. A. Shirley (LBL-U.of
Calif.), U. E. Becker, H. G.
Kerkhoff (Tech. U. Berlin & LBL),
Core-Level Photoelectron And
Auger Shape-Resonance Phenomena In
CO,CO(2),CF(4) And OCS.
Submitted to Chem. Phys.(1983).

Truesdale, C. M., P. H. Kobrin,
D. W. Lindle, D. A. Shirley
(University of Calif.-LBL), S.
Southworth (National Bureau of
Standards & LBL),
Photoelectron Angular
Distributions Of The N(2)O Outer
Valence Orbitals In-The 19-31 eV
Photon Energy Range.
J. Chem. Phys.
79(12)7117-7123(1983).

Vanderheyden, J.L., A. R.
Ketring, K. Libson, P. Motz, R. C.
Elder, E. Deutsch (University of
Cincinnati), M. J. Heeg (U. of
Oklahoma), R. Whittle (Penn State
U.),
Snythesis And Characterization
Of Cationic Technetium Complexes Of
1,2-Bis(dimethylphosphine) ethane
(DMPE)....
Inorg. Chem.(1984).

van Zon, J.B.A.D., D.C.
Koningsberger, H.F.J. van't Blik,
R. Prins (Eindhoven University of
Technology), D. E. Sayers (North
Carolina State University),
An EXAFS Study Of A Highly
Dispersed RH/Al(2)O(3) Catalyst:
Rh(o)-Rh(n+) Species In Metal
Crystallites.
Submitted to J. Phys. Chem.
(1983).

Via, G. H., J. H. Sinfelt (Exxon
Res. & Eng.), G. Meitzner (Stanford
University), F. W. Lytle (The
Boeing Co.),
Extended X-Ray Absorption Fine
Structure Of Highly Dispersed
Rhodium Catalysts.
J. Chem. Phys. 79,
03,1527-1529(1983).

Warburton, W., Z. Rek (SSRL), T.
Barbee (Stanford U.),
Performance Tests On Layered
Synthetic Microstructures (LSM's)
For X-Ray Optical Elements.
X-Ray Microscopy by
Springer.Verlag, NY(1984).

Winick, H., R. Boyce, Brown. G.,
N. Hower, T. Pate (SSRL, Stanford
U.), Z. Hussain (LBL, U. of
Calif.), E. Umbach (Tech. U.
Munchen & SSRL),
Undulator Studies At SSRL.
Nucl. Instr. & Meth.
208,127-137(1983).

Winick, H., H. Wiedemann, I.
Lindau, K. Hodgson, J. Cerino, A.
Bienenstock (SSRL-Stanford U.), K.
Halbach (SSRL & LBL), R. Bachrach
(Xerox PARC),
An All Wiggler And Undulator
Synchrotron Radiation Source.
IEEE Trans. Nucl.
Sci.,30,04(August,1983).

Wong, J., R. P. Messmer, D. M.
Maylotte (General Electric), F. W.
Lytle (Boeing Company),
K-Edge XANES Spectra Of Selected
Vanadium Compounds.
Submitted to J. Chem.
Phys.(1984).

Wong, J. , D. M. Maylotte
(General Electric), F. W. Lytle
(Boeing Company), G. Via (Exxon
Research & Eng.),
Nature Of V In Crude Oil.
Submitted to Fuel(1984).

Wong, J., (General Electric),
Method Of Fabricating Large-Area
X-Ray Filters.
Submitted to Nucl. Instr. &
Meth.(1983).

Wong, J., D. M. Maylotte, R. L.
St.-Peters (General Electric), F.
W. Lytle, R. B. Greegor (The Boeing
Company),
EXAFS & XANES Investigation Of
Trace V & Ti In Coal.
Springer Series in Chem.
Phys.27,206(1983).

Wong, Joe, (GE Res.), H. H.
Liebermann (Allied Chemicals),
EXAFS & XANES Studies Of Glassy
Ni(66)B(33): A Multi-Shell
Modelling Of The Ni-Ni
Distribution.
Phys. Rev. B. in press(1983).

Yachandra, V. K., T. G. Spiro (Princeton University), Linda Powers (Bell Laboratories).
X-Ray Absorption Spectra And The Coordination Number Of Zn And Co Carbonic Anhydrase As A Function Of pH And Inhibitor Binding.
J. Amer. Chem. Soc. 105,6596(1983).

Yeh, J. J., J. Nogami, G. Rossi (Stanford U.), I. Lindau (SSRL-Stanford U.), I. Abbati, B. DeMichelis (Inst. di Fisica di Milano).
Resonance Of 4f Partial Photoionization Cross Section Of Yb and Eu Near The 5p Threshold.
J. Vac. Sci. Tech., to be published(1983).

Zeman, H. D., E. B. Hughes, L. C. Finman, R. Hofstadter, A. Hudson, J. N. Otis, J. Rolfe (Stanford University), D. C. Rubenstein, R. S. Harrison, A. C. Kernoff (Stanford U. School of Medicine), A. C. Thompson (U. of Calif-LBL), G. S. Brown (SSRL-Stanford U.).
Evaluation Of Synchrotron X-Rays For Transvenous Coronary Angiography.
Nucl. Instru. & Meth. to be published (1984).

Zeman, H. D., E. B. Hughes, J. N. Otis, J. Rolfe (Stanford University), A. C. Thompson (U. of Calif-LBL).
Rotating X-Ray Collimating Slit For Line-Scan Dual-Energy Medical Imaging.
Proc. IEEE Nucl. Sci. Symposium, Oct.1983, San Francisco.

Zurcher, P., R.S. Bauer (Xerox PARC).
Photoemission Determination Of Dipole Layer And VB-Discontinuity Formation During The MBE Growth Of GaAs On Ge(110).
J.Vac. Sci. Tech. A1, 695(1983).

XIV ACTIVE SSRL PROPOSALS BY RESEARCH AREAS

Listed below are the SSRL proposals active in this reporting period listed by the appropriate general area of research which they represent. Some proposals are listed more than once. The number of eight hour shifts used by each research area is also indicated. These shifts encompass the time period February 23 to December 23, 1983.

IONIZATION PROPERTIES OF SMALL MOLECULES (CO, O_2, N_2, H_2, CO_2) (Shifts Used 168)

523Vp	D.A. Shirley	(University of California)	VUV and Soft X-ray Spectroscopy of Gases, Solids and Surfaces
599Vp	M.L. Knotek	(Sandia National Laboratories)	Photon-Stimulated Desorption and Auger Spectroscopy
736Vp	V. Rehn	(Michelson Laboratory)	MLSRP Research on Bulk and Surface EXAFS of Light Atoms

STRUCTURAL AND ELECTRONIC PROPERTIES OF MICROSTRUCTURES (Shifts Used 485)

582Vp	R. Bachrach	(Xerox-PARC)	Relationship of Atomic and Electronic Structure of Semiconductor Surfaces and Interfaces
611Mp	T.W. Barbee	(Stanford University)	Layered Synthetic Microstructure Characterization and Research Program
614Vp	I. Lindau	(Stanford University-SSRL)	The Electronic Structure of Metal Surfaces, and Overlayers on Metals
616Vp	I. Lindau	(Stanford University-SSRL)	The Electronic Structure, Chemistry, and Fermi Energy Pinning of Semiconductor Surfaces
636V	J.W. Allen	(Xerox-PARC)	X-ray Photoemission Studies of 2p Core Levels in Mixed Valent Rare Earth Materials
652Vp	R.S. Bauer	(Xerox-PARC)	Imperfections and Formation of Semiconductor Interfaces
689V	R.S. Stanley	(Univ. of California-LA)	Electronic Structure of Epitaxial Monolayer Films
701Vp	M.H. Hecht	(Jet Propulsion Lab)	The Effect of Many-Electron and Solid State Phenomena on Partial Photoionization Cross Sections
737Vp	V. Rehn	(Michelson Laboratory)	MLSRP Research in the Surface Chemistry of Electronic Materials
738Vp	V. Rehn	(Michelson Laboratory)	MLSRP Research on Cryogenic Molecule Films
744Vp	I. Wagner	(Exxon)	Photoelectron Spectroscopy of A-SiH_x and of Heterojunctions of A-SiH_x with Other Semiconductors
756V	R.D. Bringans	(Stanford University-SSRL)	Hydrogen Interaction with the GaAs(111) Surface
757V	D.G. Stearns	(Stanford University)	Time-Resolved Photoluminescence Decay in Hydrogenated Amorphous Silicon
763V	R.Z. Bachrach	(Xerox-PARC)	Study of Surface Reconstruction During Metal-Semiconductor Interface Formation: Si, GaAs, and ZnSe
764V	R.Z. Bachrach	(Xerox-PARC)	Study of Surface Phase Transitions and Surface Melting

771V	L. Braicovich	(Inst Di Fis. Del Polit Di Milano)	Study of the Formation of Rare Earth Elemental Semiconductor (Ge,Si) Compounds and Interfaces
772V	L. Braicovich	(Inst Di Fis. Del Polit Di Milano)	Solid State and Chemical Bonding Effects on the Cross Sections for Photoionization

PROPERTIES OF ULTRA-THIN LAYERS AND SMALL CLUSTERS

(Shifts Used 662)

523Vp	D.A. Shirley	(Univ. of California-LBL)	VUV and Soft X-ray Spectroscopy of Gases, Solids and Surfaces
528Vp	P.H. Citrin	(Bell Laboratories)	SEXAFS Studies of Adsorbates on Single Crystal Semiconductors
579V	R.C. Baetzold	(Eastman Kodak Co. Rsch. Lab)	Chemisorption Study of Surface Core Level Binding Energies for Pt Surfaces
599Vp	M.L. Knotek	(Sandia National Lab)	Photon-Stimulated Desorption and Auger Spectroscopy
614Vp	I. Lindau	(Stanford University-SSRL)	The Electronic Structure of Metal Surfaces, and Overlayers on Metals
625V	I. Lindau	(Stanford University-SSRL)	Electronic Structure of Ultrathin Transition Metal Overlayers
635Mp	J.E. Rowe	(Bell Laboratories)	EXAFS Studies of Thin-Metal-Silicides and their Interfaces
682Vp	J.W. Allen	(Xerox-PARC)	Resonant Photoemission Studies of Narrow Band Materials
684V	G.M. Rothberg	(Stevens Inst. of Technology)	Spin Polarized Photoelectron Studies of Magnetism in Solids (SPEXAFS)
686Mp	M.E. Leonowicz	(Exxon)	X-ray Structure Determinations from Crystals Less than 20 Microns in Diameter
689V	R.S. Stanley	(Univ. of California-LA)	Electronic Structure of Epitaxial Monolayer Films
695M	R.A. Dalla-Betta	(Stanford University)	X-ray Absorption Investigation of Gold Clusters
701Vp	M.H. Hecht	(Jet Propulsion Lab)	The Effect of Many-Electron and Solid State Phenomena on Partial Photoionization Cross Sections
702Mp	W. Schulze	(Fritz-Haber-Institut)	EXAFS and XANES Studies of Matrix-Isolated Metal Clusters
722M	T.I. Morrison	(Argonne National Lab)	X-Ray Absorption Studies of Rare Gas Matrices
746M	E.F. Skelton	(Naval Research Lab)	Composition Studies of ThF_4 Thin Films
766M	R.A. Scott	(University of Illinois)	Structure Determination by XAS. Some Intriging Fe-S and Co-S Clusters
771V	L. Braicovich	(Inst. Di Fis. Del Polit Milano)	Study of the Formation of Rare Earth Elemental Semiconductor (Ge,Si) Compounds and Interfaces
772V	L. Braicovich	(Inst. Di Fis. Del Polit Milano)	Solid State and Chemical Bonding Effects on the Cross Sections for Photoionization

793M	K. D'Amico	(Brookhaven National Lab)	X-ray Studies of Atomic Microclusters
796M	R.M. Suter	(Carnegie-Mellon University)	Studies of Interfacial Reactions in Thin-Film Couples

KINETIC PROCESSES IN LASER MATERIALS

(Shifts Used 11)

609Vp	R.N. Zare	(Stanford University)	Polarized Fluorescence Spectroscopy of Photofragments and Photoions
627Vp	W.C. Walker	(Univ. of California-SB)	VUV Condensed Matter Spectroscopy
786Vp	D. C. Lorents	(SRI International)	Spectroscopy and Kinetics of Excited Gases

LITHOGRAPHY AND MICROSCOPY

(Shifts Used 52)

643V	R. Tatchyn	(Stanford University)	The Heat Loading Capabilities of Ultrafine Transmission Grating Structures
692V	P.L. Csonka	(University of Oregon)	Fabrication of Superfine Holographic Diffraction Gratings with Synchrotron Radiation
727Vp	E. Kallne	(Smithsonian Astrophysics Obs.)	Optical Constants in the X-Ray Region Using Transmission Gratings
728Vp	E. Kallne	(Smithsonian Astrophysics Obs.)	X-Ray Diffraction Properties of Transmission Gratings and Zone Plates
778V	L. Golub	(Smithsonian Astrophysics Obs.)	X-ray Test of Multilayer Coated Optics

STATIC PROPERTIES AND DYNAMIC PROCESSES OF CHEMISORBED GASES

(Shifts Used 395)

523Vp	D.A. Shirley	(Univ. of California-LBL)	VUV and Soft X-ray Spectroscopy of Gases, Solids and Surfaces
528Vp	P.H. Citrin	(Bell Laboratories)	SEXAFS Studies of Adsorbates on Single Crystal Semiconductors
599Vp	M.L. Knotek	(Sandia National Laboratories)	Photon-Stimulated Desorption and Auger Spectroscopy
654V	C.S. Fadley	(University of Hawaii)	Adsorbate Core-Level Photoelectron Diffraction at High Energy
655V	E. Umbach	(Technische Univ. Muenchen)	Angle Resolved Auger Fine Structures of Adsorbed Molecules
668V	R.H. Stulen	(Sandia National Laboratories)	Valence Excited Photon-Stimulated Desorption: Hydrogen on Transition Metal Surfaces
729V	C.R. Brundle	(IBM Research Laboratory)	Photoemission Studies of Oxygen Adsorbed on W(100) and (110) Surfaces
733Vp	E.I. Solomon	(Stanford University)	UPS Studies of the Coordination Chemistry of Metal Oxide and Chloride Surfaces
736Vp	V. Rehn	(Michelson Laboratory)	MLSRP Research on Bulk and Surface EXAFS of Light Atoms
737Vp	V. Rehn	(Michelson Laboratory)	MLSRP Research in the Surface Chemistry of Electronic Materials
756V	R.D. Bringans	(Stanford University-SSRL)	Hydrogen Interaction with the GaAs(111) Surface

767V	B.B. Pate	(Stanford University)	H^+ Desorption by Valence Excitation of Diamond:Hydrogen

STRUCTURE AND FUNCTION OF HOMO- AND HETEROGENEOUS CATALYSTS (Shifts Used 113)

471Mp	D.R. Sandstrom	(Washington State University)	Investigation of Support Effects Chemisorption, and Surface Disorder in Catalysts by X-ray Absorption Spectroscopy
474Mp	J.H. Sinfelt	(Exxon)	Structural and Electronic Properties of Dispersed Metal Catalysts
547M	C.A. Mims	(Exxon)	X-ray Absorption Studies of Alkali Gasification Catalysts
598Mp	M. Boudart	(Stanford University)	In Situ Characterization of Platinum Fuel Cell Working Electrocatalysts
628M	D.G. Castner	(Chevron Research Co.)	X-ray Absorption Studies of Cobalt-Molybdenum Compounds and Catalysts
646M	T.I. Morrison	(Argonne National Laboratory)	EXAFS Characterization of Metal-Zeolite Catalysts for Indirect Coal Liquifaction
688M	R. Prins	(Eindhoven Univ. of Technology)	Structural and Electronic Properties of Supported Bimetallic Catalysts
693M	R.A. Dalla-Betta	(Stanford University)	In Situ Characterization of Fisher-Tropsch Catalysts
696M	R.A. Dalla-Betta	(Stanford University)	In Situ Characterization of Hydroprocessing Catalysts by X-ray Absorption Spectroscopy
718M	R.A. Dalla-Betta	(Stanford University)	Characterization by XAS of Burwell-Type Catalysts for $CO-H_2$ Reactions
768M	J.F. Brazdil	(Standard Oil Company)	X-ray Absorption Study of Bismuth Molybdate Catalysts
775M	M. Mehicic	(Standard Oil Company)	X-ray Absorption Spectroscopy Study of the Binary Molybdate Catalysts $A_xB_{2-x}(MoO_4)_3$
777M	R.A. Scott	(University of Illinois)	XAS Studies of Supported Catalysts, Mo-Ir Clusters on Alumina
783Mp	D.G. Castner	(Chevron Research Company)	X-ray Absorption Studies of Platinum Zeolite Catalysts
791Mp	G.H. Via	(Exxon)	X-ray Absorption Studies of Strong Metal Support Interactions

STRUCTURE OF METAL, METAL OXIDE AND SEMICONDUCTOR SURFACES AND THEIR INTERACTIONS WITH SMALL MOLECULES (Shifts Used 45)

631Mp	J. Stohr	(Exxon)	Photon Stimulated Ion Desorption: Mechanistic Studies and Application to Surface Chemistry and Crystallography
681M	C.R. Helms	(Stanford University)	Impurity Bonding in Semiconductors
685M	R.W. Schwartz	(Michelson Laboratories)	Adsorbed Lanthanide Complexes as Probes of Molecular Surface Topology
715M	G.S. Cargill	(IBM Watson Research Center)	EXAFS for Heterojunction Interfaces: Ni-on-Si Schottky Barrier Junctions

735Mp	J. Stohr	(Exxon)	Surface EXAFS Studies of Solid-Solid Interface Formation Schottky Barriers
776M	K.O. Hodgson	(Stanford University)	Molecular Models for Metal-Oxide Surface Interactions

STRUCTURE OF GENERAL CHEMICAL COMPOUNDS THROUGH EXAFS

(Shifts Used 167)

656M	C.P. Wong	(ERC, Western Electric Co.)	EXAFS Studies of Some Lanthanide Prophyrin and Transistion Metal Complexes
674M	L.J. Altman	(Mobil Research & Development)	Study of the Nickel Containing Compounds in Petroleum
675M	S.S.P. Parkin	(IBM Research Laboratory)	X-ray Absorption Studies of Organic Linear Chain Conductors
676M	J.V. Acrivos	(San Jose State University)	Study of Metal Ammonia Systems
678Mp	D.H. Maylotte	(General Electric)	Trace Element Sites in Coal and Other Fossil Fuels
690Bp	R.C. Elder	(University of Cincinnati)	Technetium Radiopharmaceutical Imaging Agents: EXAFS and Edge Studies
700M	J.E. Hahn	(Stanford University)	Structures of Mercury (II) Complexes in Solution
704M	R. Bauer	(Risoe National Laboratory)	Metal-Metal Distances by EXAFS in Dinuclear Transition Metal Complexes
717M	J.G. Gordon	(IBM Research Laboratory)	Study of EXAFS from Wet Electrode Surfaces
721M	D. Sandstrom	(Washington State University)	Study of Strong Electrolytes by X-Ray Spectroscopy at the Cl K-edge
723B	I.C. Baianu	(University of Illinois	X-Ray Diffraction Studies of Magnetically Oriented Photosystem II Particles and Thylakoids
734M	N.R. Farrar	(Raychem Corporation)	SAXS from Unfilled and Filled Polymer Resins
754Mp	R.B. Greegor	(Boeing Company)	X-ray Spectroscopic Investigation of Metamict Minerals
755M	T.P. Russell	(IBM Research Laboratory)	Phase Separation of Low Molecular Weight Polymer Mixtures
758M	D. de-Fontaine	(Univ. of California-Berkeley)	Three-Radiation Analysis of Spinodal Decomposition
765M	P.A. Montano	(West Virginia University)	EXAFS Study of Iron Sulfides and Ni-Mo During Coal Liquefaction
770M	B. McQuillan	(GA Technology)	Studies of the Vanadium Site Symmetry in Various Oxides and Oxyanions
780M	B.M.L. Rao	(Exxon)	Study of Precipitate Nucleation and Molecular Association in Asphaltene Solutions

MULTIPLE WAVELENGTH IMAGING

(Shifts Used 22)

456Bp	E.B. Hughes	(Stanford University)	Iodine Dichromography with Monochromatic X-ray Beams for Angiography

PROTEIN STRUCTURES AND FUNCTIONS THROUGH DIFFRACTION STUDIES IN THE CRYSTALLINE STATE (Shifts Used 21)

634B	W. Hendrickson	(Naval Research Laboratory)	Anomalous Scattering Crystallography of Lamprey Hemoglobin
651Bp	R.P. Phizackerley	(Stanford University-SSRL)	Protein Crystallographic Structural Studies Using Anomalous Scattering
680Bp	R. Almassy	(Univ. of California-LA)	The Structure of Glutamine Synthetase

DYNAMICS AND FLUZUATIONS IN BIOLOGICAL SYSTEMS (Shifts Used 100)

518Bp	J.K. Blasie	(University of Pennslylvania)	Time-Resolved Structural Studies of Integral Membrane Proteins
660B	B. Chance	(University of Pennslylvania)	Low Temperature Photolysis/ Recombination of Hemoproteins Under Conditions of Nuclear Tunneling
663Bp	H.W. Huang	(Rice University)	Protein Dynamics by Time-Resolved EXAFS and Edge Spectra
691Bp	S.G. Boxer	(Stanford University)	Time Resolved Fluorescence from Photosynthetic Models and Chlorophyll-Protein Complexes
774B	B.R. Stults	(Monsanto Company)	X-ray Absorption Studies of Phosphoryl Transfer Reactions
787B	C. Borso	(Argonne National Laboratory)	Time Resolved Small Angle Scattering Study of Deoxygenated Sickled Hemoglobin

NATURE OF MEMBRANE STRUCTURES AND MEMBRANE PROTEIN INTERACTIONS (Shifts Used 57)

645B	S. Doniach	(Stanford University)	X-ray Diffraction Studies of Immunoglobulin-Membrane Complexes
673Bp	M.P. Klein	(Univ. of California-LBL)	X-ray Absorption Studies of Manganese in Photosynthetic Systems
707B	S. Doniach	(Stanford University)	Small Angle X-ray Diffraction Studies of the Acetylcholine Receptor
731B	B. Chance	(Univ. of Pennslylvania)	Anomalous X-ray Scattering Studies of Dense Cytochrome Oxidase
748BP	H.M. McConnell	(Stanford University)	X-ray Total External Reflection Studies on Phospholipid Monolayers
759B	I.C. Baianu	(University of Illinois)	Small-Angle X-ray Scattering of Lecithin-Cholesterol Acyltransferase

STRUCTURE AND FUNCTION OF METAL-SITE IN METALLOPROTEINS AND METALLOENZYMES (SHIFTS USED 209)

490bp	E.A. Stern	(University of Washington)	X-ray Absorption Studies of Metalloproteins
559Bp	R.C. Elder	(University of Cincinnati)	EXAFS of Gold-Based Drugs Used to Treat Rheumatoid Arthritis
632Bp	B. Chance	(Univ. of Pennslylvania)	Structure-Function Relationships in Cytochrome-c Oxidases, Related Oxidases Peroxidases and Models
638B	M.P. Klein	(Univ. of California-LBL)	Effects of Chaotropic Agents on the Methionine Coordination of Ferricytochrome c
644B	K.O. Hodgson	(Stanford University)	Polarized X-ray Absorption Spectroscopy on Oriented Samples

657B	S.P. Cramer	(Exxon)	Single Crystal EXAFS of Nitrogenase
658B	E.D. Crozier	(Simon Fraser University)	X-ray Absorption Studies of Phospholipase A2
664B	M.P. Klein	(Univ. of California-LBL)	Manganese and ADP Binding to Active Site of ATPase
665B	T.G. Spiro	(Princeton University)	EXAFS Studies of Hemocyanin and Tyrosinase
672B	M.P. Klein	(Univ. of California-LBL)	X-ray Spectroscopy of Manganese Superoxide Dismutases from E. Coli & T. thermophilus
687B	J.C. Smith	(Georgia State University)	Investigations of the Rieske Iron-Sulphur Protein using Synchrotron Radiation
698Bp	K.O. Hodgson	(Stanford University)	XAS of Bioinorganic Molybdenum and Related Systems: Nitrogenase and Xanthine Oxidase
699B	K.O. Hodgson	(Stanford University)	XAS Studies on the Active Oxygen Intermediates of Heme-Containing Enzymes
703B	R. Bauer	(Risoe National Laboratory)	EXAFS Studies of the Catalytic Metal Site in Alcohol Dehydrogenase
705B	D.M. Ho	(Stanford University)	EXAFS Studies on Models of Platinum Anti-Cancer Drug/DNA Interactions
710B	B. Muhoberac	(Univ. of Texas-San Antonio)	Structural Studies of the Catalytic Center(s) of Pseudomonas Cytochrome Oxidase
730B	J. Wong	(General Electric)	EXAFS Studies of Respiratory Succinate Dehydrogenase
732B	L. Powers	(Bell Laboratories)	Calcium Edge and EXAFS Studies of Biological Molecules
761Bp	R.A. Scott	(University of Illinois)	XAS Studies on the Active Sites of Cytochrome c Oxidase
762Bp	R.A. Scott	(University of Illinois)	Structural Aspects of Iron-Sulfur Clusters in Proteins and Models
781B	K.O. Hodgson	(Stanford University)	Polarized X-ray Absorption Spectroscopy on Oriented Hemocyanins
784B	S.P. Cramer	(Exxon)	X-ray of Active Molybdenum Cofactor
785B	S.P. Cramer	(Exxon)	Mo and As EXAFS of Substrate Complexes of Arsenite-Inhibited Xanthine Oxidase
790B	D.E. Sayers	(North Carolina State Univ.)	X-ray Absorption Studies of the Protein Iron Interface in Ferritin

STRUCTURE OF AMORPHOUS MATERIALS

(Shifts Used 141)

509Mp	P.H. Fuoss	(Bell Laboratories)	Anomalous Scattering Techniques and Their Application to Disordered Systems
615Mp	F. Lytle	(Boeing Company)	Investigation of Atomic and Electronic Structure of Glass
639Mp	J.B. Kortright	(Stanford University)	Structural Studies of Amorphous Mo-Ge Alloys

650Mp	R.H. Martinson	(Lockheed Research Laboratory)	Dynamic Small Angle Scattering Experiments on Polymeric Materials
683M	J. Wong	(General Electric)	High-Content Metalloid Metallic Glasses: A Test for Polk Model
706Mp	W.K. Warburton	(Stanford University-SSRL)	Partial Structure Factor Determination in Binary Liquids by Anomalous X-ray Scattering
709M	A.Fischer-Colbrie	(Stanford University)	Structural Studies of Photo-Enhanced Diffusion of Ag in Amorphous $GeSe_2$
741M	G.E. Brown	(Stanford University)	K-Edge and EXAFS Study of Na, K, and Ca in Amorphous and Crystalline Aluminosilicates
747M	J.C. Mikkelsen	(Xerox-PARC)	Study of Vegard's Law in Pseudo-binary Solid Solutions
752M	J. Wong	(General Electric)	Bonding and Structure of Pb in Novel $PbO-PbCl_2$ Glasses Using Xanes and EXAFS
753M	J. Wong	(General Electric)	Structure and Bonding in Novel Ionic Sulphate Glasses
760M	M. Marcus	(Bell Laboratories)	Impurity-Host Interaction in Metallic-Glass Forming Systems
769M	M. Tenhover	(Standard Oil Company)	Structural Study of Ge-Sn-Se-S Glasses by X-ray Absorption Spectroscopy
788M	K. Ludwig	(Stanford University)	X-ray Study of the Structural Transition in Molten Se_xTe_{1-x}
789M	A.Fischer-Colbrie	(Stanford University)	X-ray Scattering Studies of Very Thin Disordered Layers
797M	T.I. Morrison	(Argonne National Laboratory)	P-Edge EXAFS Studies of P_xSe_{1-x} Glasses

COORDINATION OF IMPURITIES AND ALLOYING SPECIES

(Shifts Used 50)

647Mp	G.P. Huffman	(US Steel Corp. Rsch. Laboratory)	EXAFS Investigation of Problems of Interest to the Steel Industry
653M	R.W. Hoffman	(Case Western Reserve Univ.)	Structure of Electrochemically Passivated Ferrous Layers
724M	M.B. Stearns	(Arizona State University)	Radial Displacement Surrounding Solutes in Fe, Ni and Cu
725M	M.B. Stearns	(Arizona State University)	Bond-Lengths and Local Environment Studies Surrounding Mn, Rb Sr and Y Solutes in Ca F_2 and Pb F_2
726M	M.B. Stearns	(Arizona State University)	Strain Induced Effects Surrounding Impurity Cations (X = Mn,Fe,Co,Ni,Zn) in the Rutile Systems $Mn_{1-x}X_xF_2$ and $Ni_{1-x}X_xF_2$

STRUCTURES OF AND PHASE TRANSITIONS IN SURFACES AND THIN SURFACE LAYERS

(Shifts Used 269)

564Mp	P.H. Fuoss	(Bell Laboratories)	Application of X-ray Reflection-Diffraction Techniques to the Study of Disordered Interfaces
608Mp	P. Eisenberger	(Exxon)	Reflection Diffraction Scattering Program

623Mp	S.K. Sinha	(Exxon)	High-Resolution Diffraction Studies of Carbon Tetrafluoride Monolayers Physisorbed on Graphite
708Mp	S.C. Moss	(University of Houston)	Structural Studies of Ordering in Intercalates of Graphite and TiS_2
713M	D.E. Moncton	(Brookhaven National Laboratory)	High Resolution Study of Liquid Crystal Thin Films
714M	J.P. McTague	(Brookhaven National Laboratory)	X-ray Study of Two-Dimensional Melting of Submonolayer Argon Films on Pyrolytic Graphite
716Mp	P.S. Pershan	(Harvard University)	High Resolution Study of Structural Phase Transitions in Freely-Suspended Liquid Crystal Films
720Mp	M. Sutton	(M.I.T.)	Multilayer Adsorption on Graphite
739M	P.N. Sanda	(Exxon)	Structural Studies of Tungsten (100) Using Grazing-Incidence X-Ray Scattering
742Mp	P. Horn	(IBM Watson Research Center)	Multicritical Melting of Xenon on Graphite
743Mp	S. Brennan	(National Bureau of Standards)	SEXAFS/Surface Bragg Scattering Studies of Structure and Dynamics
745M	I. Robinson	(Bell Laboratories)	Nitrogen Orientation on Graphite
792M	C.R. Safinya	(Exxon)	High Resolution X-ray Studies of Freely Suspended Thin Strand Discotics

KINETICS OF STRUCTURAL CHANGES IN MATERIALS

(Shifts Used 17)

669M	M.P. Scott	(Hewlett Packard)	Real Time X-ray Topography of Oxygen Precipitation in Silicon

PHASE TRANSITIONS AT HIGH PRESSURE

(Shifts Used 0)

489Mp	R.L. Ingalls	(University of Washington)	X-ray Absorption Studies of Materials Under High Pressure
626M	E.F. Skelton	(Naval Research Laboratory)	Studies of Intercalated Solid Lubricants at Extreme Pressures and Temperatures
640M	O. Shimomura	(Nat. Inst. Inorganic Materials)	Application of EXAFS and Diffraction Using Anomalous Scattering to High-Pressure Research
719M	O. Shimomura	(Nat. Inst. Inorganic Materials)	X-Ray Absorption Study of Pressure-Induced Electronic Transition in Cesium
740M	S.B. Qadri	(Naval Research Laboratory)	Structural Studies of Ternary Chalcopyrite Semiconductors at Elevated Pressures and Temperatures
750M	A.W. Webb	(Naval Research Laboratory)	Compressibility and Thermal Expansion Under Pressure of Ni_3Sn
751Mp	S.A. Wolf	(Naval Research Laboratory)	Low Temperature and High Pressure Structural Studies of Anisotropic and Organic Conductors and Superconductors

782M	M.H. Manghnani	(University of Hawaii)	In Situ High Pressure-High Temperature X-ray Diffraction Studies for Investigation of Phase Transformations in Mantle Phases and the Equation of State of Gold: Application in Geochemistry and Geophysics

STRUCTURE OF CRYSTALLINE MATERIALS

(Shifts Used 0)

543Mp	H.L. Yakel	(Oak Ridge National Laboratory)	Determination of Site Occupation Parameters in 3d Transition Metal Phases
629M	D.R. Sandstrom	(Washington State University)	EXAFS Study of Structure in Layered Copper-Manganese Salts
649M	T.K. Sham	(Brookhaven National Laboratory)	X-ray Absorption and EXAFS Studies of $SrTiO_3$ through the 110 Degree K Cubic to Tetragonal Phase Transition
677M	J.V. Acrivos	(San Jose State University)	X-ray Absorption Studies of Layered Materials and their Intercalates
773M	J.V. Acrivos	(San Jose State University)	X-ray Diffraction and Absorption Studies of Periodic Lattice Distortions
795M	R.M. Fleming	(Bell Laboratories)	Charge-Density Waves in Linear Chain Compounds

ELECTRONIC STRUCTURE OF MATERIALS THROUGH EDGE ABSORPTION STUDIES

(Shifts Used 13)

667M	F.W. Lytle	(Boeing Company)	Investigation of Electronic Structure in Ferroelectrics by their L-Absorption Spectra
794Mp	K.O. Hodgson	(Stanford University)	X-ray Absorption Edge Structure as a Probe of Electronic Structure

FUNDAMENTAL X-RAY SCATTERING AND ABSORPTION PHYSICS

(Shifts Used 93)

562Mp	E.A. Stern	(University of Washington)	Many-Body and Chemical Effects in EXAFS
641Bp	D.H. Templeton	(Univ. of California-LBL)	Anomalous Scattering Measured by Single Crystal Diffraction
659B	B. Chance	(Univ. of Pennslylvania)	Flow Apparatus Tests of Hemeprotein Reactions at High Beam Intensities
679M	D.G. Stearns	(Stanford University)	A Systematic Study of Phase Transferability in EXAFS Using Linearized Phase Shifts
712B	S. Doniach	(Stanford University)	Anomalous Small-Angle X-ray Scattering from Solutions of Terbium-Labelled Proteins
749M	I. Freund	(Bar-Ilan University)	Parametric Down Conversion of Synchrotron X-Radiation into the Extreme Ultra-Violet

ATOMIC PHYSICS

(Shifts Used 26)

603M	G.S. Brown	(Stanford University-SSRL)	Atomic Inner-Shell Threshold Excitation Phenomena Investigated by Electron Spectroscopy
779Mp	G.S. Brown	(Stanford University-SSRL)	Gas-Phase Threshold Electron Spectrometry of Atomic Inner Shells

SYNCHROTRON RADIATION SOURCE AND INSTRUMENTATION DEVELOPMENT

(Shifts Used 15)

633M	J.V. Gilfrich	(Naval Research Laboratory)	X-ray Fluorescence Analysis Using Synchrotron Radiation
662Mp	E.A. Stern	(University of Washington)	Development of Modulation Techniques with Applications to Ferroelectrics
670Bp	A. Thompson	(Univ. of California-LBL)	Development of a Scanning X-ray Microprobe
671M	M.P. Klein	(Univ. of California-LBL)	X-ray Spectroscopy of Mn:Al_2O_3:Mg and Optical Detection of EXAFS

11.0 University of Illinois at Urbana-Champaign Center for Microanalysis of Materials

1. **What new science is being explored by this facility? What scientific opportunities are being exploited?**

Answer: The Center for the Microanalysis of Materials is an integral part of the University of Illinois Materials Research Laboratory and serves researchers at the University of Illinois as well as those working in other universities, government laboratories and in industry on a nationwide basis. The focus of the effort within the Center is to make available to this community the techniques and instrumentation for microstructural, microchemical and structural characterization which is becoming increasingly necessary in solid state physics, metallurgy, ceramics, polymers and other areas of materials science and engineering. The Center has the capability for such characterization on a scale ranging from macroscopic dimensions down to dimensions of the order of one nanometer. In materials science and engineering it is essential to know the chemical composition, crystallographic structure, and the electronic and optical properties of materials on an increasingly finer scale. The Center provides this research opportunity for a very wide range of scientists.

2. **What are this facility's unique features (i.e., not duplicated elsewhere)?**

Answer: The Center for the Microanalysis of Materials at the University of Illinois Materials Research Laboratory plays a unique role in Materials Science and Engineering in this country and in the world. It is a uniquely equipped University-based facility for the application of modern microanalysis and surface analysis techniques and equipment to the problems which are at the forefront of the field of Materials Science and Engineering. Furthermore, it is perhaps the only facility which has the multiple purpose of a) making instrumentation and techniques available to users, b) developing new analytical and microcharacterization methods and instrumentation, and c) educating graduate students in the area of microanalysis of materials.

3. **What types of research instrumentation/experimental devices are available at this facility, and what are their capabilities?**

Answer: 1. Imaging Secondary Ion Microprobe (Cameca IMS 3f, acquired 1980). Mass-analyzed images with a 0.3 micron - 400 micron lateral resolution and 50-100 A depth resolution; profiling up to 50 A/sec; to be developed by the incorporation of a second ion source.

2. Scanning Auger Microprobe (PHI 545, acquired 1973) SEM images with 3 micron resolution; ion gun for depth profiling; mass spectrometer; samples 77 - 300 K; LEED and I.S.S.

3. XPS (PHI 548, acquired 1980). 10 kV Mg X-ray source; Varian sputter gun; double-pass CMA; ESCA and Auger analysis; samples 300 - 1500 K; gas handling facilities for adsorption studies; local developments will include a cold stage and a sample preparation and tensile failure chamber. TRS-80 and floppy disc data acquisition.

4. Scanning Auger/SEM (PHI 595, acquired 1980). Scanning images with 300 A resolution; scanning Auger images with 700 A resolution; X-ray microchemistry (Kevex system with thin window detector). In situ fracture.

5. X-ray Diffraction. There are two rotating anode sources (Elliott 15 kW high brilliance source; Rigaku 12 kW) and several conventional x-ray sources. They are fitted with the following equipment:

a) Huber four-circle diffractometer, LSI-11 computerized data acquisition and helium sample stage.

b) small angle scattering camera (20') with area detector

c) EXAFS (transmission and fluorescence)

d) high-resolution triple-axis diffractometer with hot and cold stages: computerized

e) 2 Lang topography cameras

f) a topographic system that needs no mechanical scanning

g) 2 automatic powder diffractometers

h) a Laue camera, single crystal cameras and other standard equipment.

6. 300 kV Transmission Electron Microscope (Phillips EM430, to be acquired 1984). This microscope, of a new generation operating at intermediate voltages, will be equipped with EDX and EELS. It will be compatible with all the equipment for the EM420 and EM400T.

7. 120 kV Transmission Electron Microscope (Phillips EM420; acquired 1982). This instrument is fitted with Energy Loss Electron Spectroscopy (EELS) and a secondary electron detector as well as Energy Dispersive X-ray analysis (EDX). This instrument has been developed by the addition of increased flexibility in the scanning and alignment system. In addition it has all the facilities of the EM 400T.

8. 120 kV Transmission Electron Microscope (Phillips EM400T, acquired 1980). Fitted with twin-lens and EDX analytical capability. Hot and cold (liquid helium and liquid nitrogen) stages are available.

9. Scanning Electron Microscope (JEOL JSM-35C, acquired 1980). 50 A resolution, EDX fitted, general purpose SEM. Facility to produce channeling patterns.

10. Scanning Electron Microscope (JEOL JSM U3, acquired 1970). 200 A resolution, primitive EDX facility available, hot stage, cold stage, and tensile stage available. This machine is generally given over to long-term, single-user operation e.g., for beam-writing experiments. A Kossel camera has been fitted.

11. Scanning Transmission Electron Microscope (VG HB5, acquired 1978). This STEM produces a 5 A electron probe and can carry out EDX and EELS analysis down to about 20 A spatial resolution.

12. Rutherford Backscattering (in-house construction). The backscattering of He^4 ions from the Van de Graaff accelerator are used to study the composition and symmetry of samples, with depth profiling on the scale of 40 A resolution in depth. These tests are non-destructive. The equipment, including facilities for channeling studies, has now been built.

Two electron microprobes, one computerized, are housed in the Geology Department and maintained with the aid of MRL personnel under reciprocal agreements that can be extended to external users.

Related characterization facilities that are not "microscopic" are also associated with the Center. These include optical microscopes, a spark source mass spectrometer, a surface profiler, a microhardness tester, etc.

4. **What have been the facility's research highlights for the period FY 1981 - present, and what are anticipated for the remainder of FY 1984 and FY 1985?**

Answer: As discussed in Question 1 above, the role of the Center in making state-of-the-art facilities available to a wide range of researchers has allowed the personnel associated with the Center to take part in a large number of exciting and significant scientific developments. These are more properly reviewed by the reports of the principal scientist who lead the research efforts. In the following we will list only those things which have been directly associated with the in-house research component of the Center's operation.

1. Development of the ability to carry out microlithography with a 10 - 20 A resolutions and the development of an understanding of the mechanisms by which these patterns can be developed. The scale of pattern development which has been demonstrated at the Center is a factor of one thousand smaller than is presently used commercially.

2. Development of the technique of zone axis electron diffraction which allows the study of surface structure in the TEM.

3. Increased understanding of the mechanisms of sputtering and ion yields in metals and semiconductors based in part on the work in the Center has led to placing the SIMS method of analysis on a sounder scientific basis. The work at the Center has led to understanding the effects of matrix chemistry on ion yields, an understanding which is fundamental to the entire technique.

4. Understanding of the mechanisms of ion desorption by electrons and by ion beams, particularly understanding the energy spectrum of the secondary ion emission, has developed as a result of studies in the Center.

5. Research on ion beam effects in the Center has led to understanding ion beam mixing and ion induced diffusion; particularly the effects of these processes on interfaces. These effects are important not only for the use of ion beams for microanalysis but also for understanding the use of ion beams in materials processing and semiconductor doping.

6. The addition of a cathodoluminescence detection system to one of the scanning electron microscopes has greatly extended its usefulness for studies of semiconductors, insulators and minerals. It will allow the measurements of the optical properties of regions of less than one micrometer in diameter.

7. The development of a Rutherford backscattering system with its ability to be used for channeling experiments will enhance our ability to carry out thin film and modulated structure analysis. We expect to produce exciting new results in these areas as well as in the area of grain boundary structure and chemistry.

5. **What facility changes and additions have occurred or are anticipated for the period FY 1981 - FY 1985?**

Answer: Since the Center for the Microanalysis of Materials was begun in 1981, most of the structure and instrumentation can be included in a response to this question. The instrumentation, with some exceptions has been developed, purchased and installed in this period.

In order that the Center fulfill its primary function, that of providing access to state-of-the-art instrumentation for a wide range of users, it will be necessary to develop and update the facilities of the Center continuously. It is anticipated that one major instrument will require replacement each year in the steady state.

6. **For the period FY 1981 - FY 1985, please provide actual and estimated budget profiles for operations, in-house research, out-of-house research, other operating expenses, Capital Equipment, General Plant Projects, In-House Energy Management, and any other specific construction projects attributable to the facility. Please indicate the source of these funds (i.e., Materials Sciences, Chemical Sciences, Nuclear Sciences, Applied Mathematical Sciences, other BES, Medium Energy Nuclear Physics, Heavy Ion Nuclear Physics, Low Energy Nuclear Physics, High Energy Physics, etc.).**

Answer:

(B/A in thousands)

	1981	1982	1983	1984	1985
SOURCE OF DOE FUNDS					
OPERATING EXPENSES					
D.O.E. MATERIALS SCIENCE	$224	$255	$325	$330	$350
MAJOR EQUIPMENT ACQUISITIONS					
D.O.E. MATERIALS SCIENCE	22	495	120	0	150
TOTAL	$246	$750	$445	$330	$500

7. **How much funding for FY 1981 - FY 1985 has been or is expected to be provided by other federal agencies such as the National Science Foundation, by State agencies, by foreign institutions, or by private sources?**

Answer:

	(B/A in thousands)				
	1981	1982	1983	1984	1985
OTHER GOVT. AGENCIES	178	314	507	450	415
PRIVATE SOURCES	22	23	24	30	35

8. **For the period FY 1981 - FY 1985, please provide actual and estimated staffing levels.**

Answer: The total staffing at the Center, of which the Materials Sciences program funds are about one half, is as follows:

FY 81 - 12.5 FTE
FY 82 - 12.5 FTE
FY 83 - 12.5 FTE
FY 84 - 12.5 FTE
FY 85 (est.) - 12.5 FTE

9. **What is the actual and estimated facility utilization for the period FY 1981 - FY 1985? What would be defined as "full" utilization of the facility?**

Answer: The following instruments are generally used in cooperation with a Center staff member until the user has a good deal of experience on the instrument.

Secondary Ion Mass Spectrometer
Scanning Auger Spectrometer
X-ray Photoelectron Spectrometer

The following instruments are generally user operated after a training period.

Transmission electron microscopes
Scanning electron microscopes
X-ray equipment
Scanning transmission microscopes

Full utilization is defined as 40 hours per week as the Center is funded for a one shift operation. On those instruments which are primarily user operated the utilization also occurs in the off hours.

AVERAGE ACTUAL USAGE (HOURS/WEEK)	
Transmission electron microscopes (each machine)	60
Scanning transmission microscope	20
Scanning electron microscope	30
X-ray equipment	10 - 110
(the variable figure results from the varied use on the different units)	
Secondary ion mass spectrometer	33
Scanning Auger spectrometer	38
X-ray photoelectron spectrometer	23

The usage on some of these instruments has been rising rapidly as they become integrated into the Center's operation. For example, the X-ray photoelectron spectrometer usage listed above reflects the period when it was first being developed as a facility instrument. Its current usage is over 40 hours per week. The above averages are taken over a multiple year period.

10. **For the period FY 1981 - FY 1985, how many experiments will have been started, continued, and completed?**

Answer: Most of the experiments which are carried out in the facility are originated and developed by the facility users. As explained above, these are a diverse group. The number of experiments is approximately equal to the number of users.

The average number of users per year is 200.
The average number of new users per year is 70.

11. **What is this facility's user policy?**

Answer: This facility is not a DOE-owned facility. The Center for the Microanalysis of Materials operates within the structure of the Materials Research Laboratory under the direction of the Director of the MRL. The policies which govern its operation are set by the Facility Committee and are approved by the MRL Director. Since the Center operates primarily for the benefit of its users, the policies which govern their access are kept simple and are flexible.

The present policies may be summarized as follows:

a) Use of the facility requires approval of the Facility Committee which has delegated its authority of approval to the operational director of the laboratory in routine cases. Non-routine cases are referred to the Facility committee for decision.

b) Access to the instruments requires that the user demonstrate competence in using the equipment. In the event that such competence does not exist, instruction in the use of the equipment can be arranged.

c) Scheduling of time on the instruments is arranged by the section leaders in the Center. In the case of any disputes these will be brought to the Facility Committee for adjudication.

d) Access to the facility for non-MRL users is arranged by the operational director of the lab on the basis of discussions with the prospective users. When possible, interactive research cooperation between the outside users and the facility personnel will be offered.

e) Use of the facility by non-MRL, non-DOE users is restricted to projects which have a research component. Routine analysis which could be carried out by commercial facilities are not allowed.

f) All users are required to pay a fee the magnitude of which depends on the instrument used and the organization to which the user belongs and the source of research support. The magnitude of the fee is determined by the requirement that the operating costs of the instruments be recovered from the fees.

g) In the event that a prospective user has a meritorious project but cannot pay the user fee, he may petition the Facility Committee which has the authority to assign free time on the instrument. The intent of this policy is to prevent the application of the fee from interfering with the use of the instruments for desirable research applications.

12. **For the period FY 1981 - FY 1985, how much reimbursable research has taken place or is estimated to take place? What revenues have been involved?**

Answer: In accord with the operating policy of the Center all research use of the facilities is on a reimbursable basis. The contract or organization which supports the research is asked to pay the usage fee which varies according to the instrument used. These fees are set at a level to meet the operating costs of the instruments.

Approximately 20% of the usage of the Center is by non-MRL programs which may be from other University of Illinois contracts, other University contracts, from Federally supported research facilities or from industrial firms. A partial listing of these outside users for a six month period is given below.

Northwestern University (B. Wessels, DOE): Radiation damage and native defect properties in zinc selenide.

Northwestern University (B. Wessels, NSF): Defects in indium phosphide.

American Philips Research (A. E. Morgan): Dopant segregation coefficients at the Si/SiO_2 interface.

Arizona State University (I.S.T. Tsong, DOE): Ion sputtering yields of Si and N.

Lawrence Livermore (C. Price, DOE): N_2 diffusion profiles in steels and vanadium.

Crane Naval Labs (D. File): Photocathode defects

U. S. Army ERADCOM (J. Oberstar): Penetration of contact elements. Diffusion of Be implants in doped InP.

Oxford University (C. J. Humphreys): Radiation damage in the beta-aluminas.

Sandia National Labs (B. Tuttle): Intergranular phases in ZnO varisters.

Oak Ridge National Laboratory (J.H. Schneibel): Sulphur precipitation in Ni-Cr alloys.

Argonne National Laboratory (J. Routbort): Oxygen diffusion in transition metal oxides.

University of Michigan, Ann Arbor (L.F. Allard, DOE): Microstructure of binder phases in ceramic interfaces.

Michigan State (Dr. Subramanian): Composition variation in spinodal decomposition.

Texas A&M University (J. Bockris): Structure of platinum deposits on semiconductors.

Argonne National Laboratory (R. Averbach): Ion beam mixing and enhanced diffusion.

California Institute of Technology (M. A. Nicolet): Influence of ion-implanted F and Cl on Si expitaxial re-growth.

American Philips Research (M.E. Lunnon): Rapid annealing of boron implants in silicon.

EG and G (Idaho Falls): Preferred orientation in welds in stainless steels.

Cummins Engine Co. (G.L. Starr): Structures of ceramic coatings on metals.

13. **What is the mechanism by which specific research proposals for experiments at the facility are considered?**

Answer: Members of the MRL are requested to discuss their proposed experiment with the operational director of the laboratory who screens the use for suitability and attempts to facilitate interactions between the research group and suitable facility personnel. In the case of long time users of the facility this type of interaction generally arises in a natural fashion. In general all applications by MRL personnel which are judged to be suitable are accepted. Non-MRL users are treated in a similar fashion with an additional element of screening which ensures that the desired use is research oriented and does not conflict with the prohibition against use of the Center for routine non-research oriented programs.

All cases of dispute are brought to the Facility Committee for discussion and decision.

14. **How many research proposals have been submitted over the past five years, and how many of these have been approved?**

Answer: Since a formal proposal procedure is not used we do not have good statistics concerning the number of proposals received. In an average year the Center will have approximately 200 different users. Of these about 20% will be from non-MRL research groups.

The fraction of proposals for use of the facility which have been accepted is not documented because of the manner in which the facility operates. We attempt to meet the needs of all prospective users who approach us with a meritorious proposal and most of the prospective users are accommodated.

15. **How many university personnel (i.e., faculty and students) have utilized the facility over the past five years?**

Answer: Information concerning this usage is available for the past two years during which the Center was in full operation. During this period the number of University users was about 350.

16. **How many industrial researchers have utilized the facility over the past five years?**

Answer: During the past two years in which the facility has been in full operation, the number of industrial users has been 20.

17. **How many researchers from foreign institutions have utilized the facility over the past five years?**

Answer: During the past three years, we have had three foreign users per year. All have been from NATO countries.

18. **How many researchers from other agencies have utilized the facility over the past five years?**

Answer: The average number of facility users from other Federal agencies is 6 per year. In addition, interactive research carried out by the facility personnel with researchers at Federally supported laboratories accounts for a considerably greater usage.

19. **What are the future development possibilities for this facility (including research instrumentation/experimental devices), what plans are being made to exploit these possibilities, and what are the budgetary implications?**

Answer: In order that the Center facilities be maintained at the cutting edge of science it will be necessary to continue our instrument development and modernization program. Since the Center primarily serves the need of researchers in a wide range of disciplines and institutions our development will reflect the increasing demand and need for the types of instrumentation and interactions which we can provide. We would project a modest growth in response to the increased needs and opportunities for new techniques and new science. It is certain that as Materials Science and Engineering develops there will be increased needs for the types of science which the Center can provide and support. Maintenance of our present program will require that one major instrument be replaced each year.

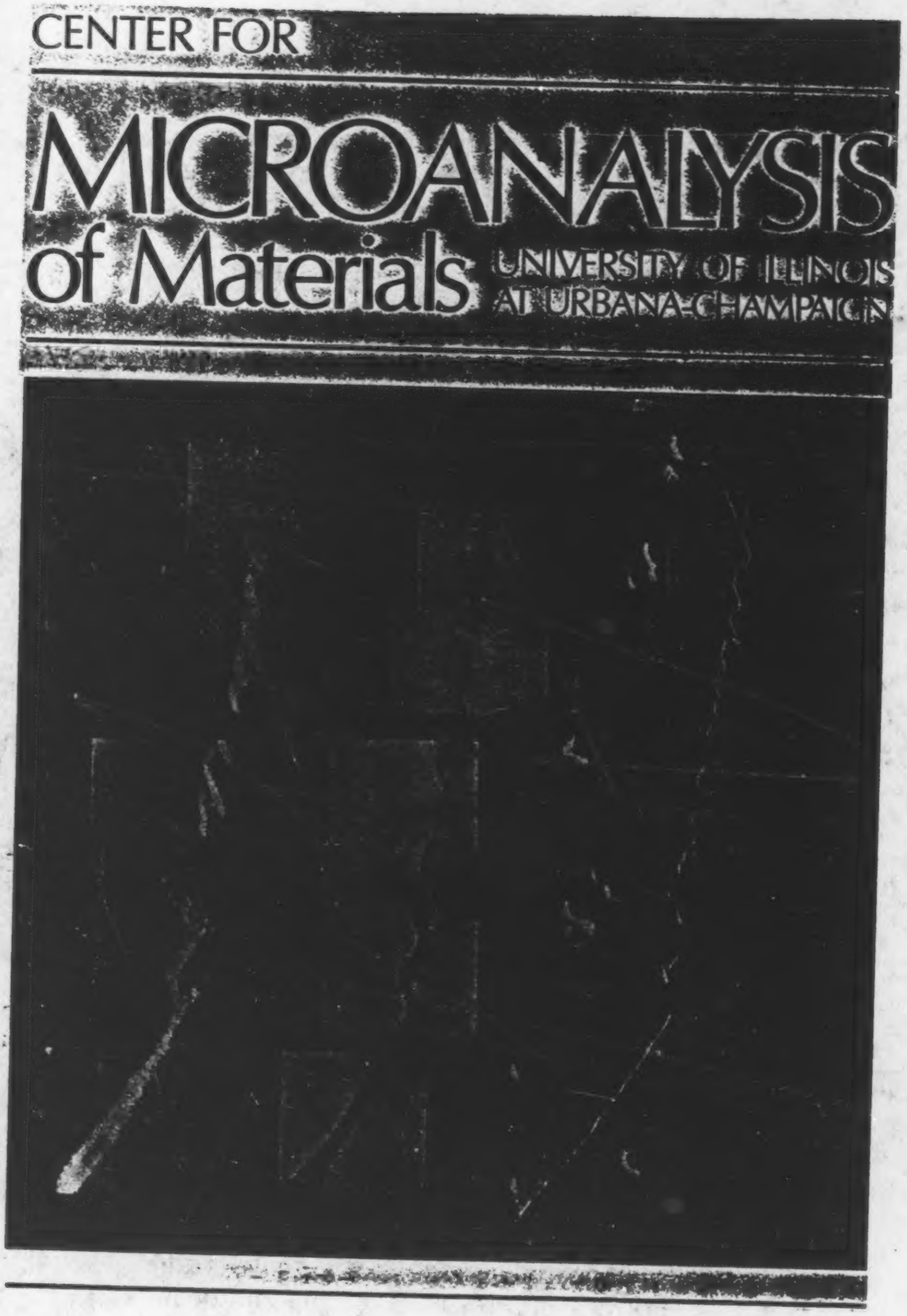
We expect that overall size of the facility will remain about constant and that the personnel level will remain constant.

New instrumentation is planned in the area of environmental cell TEM studies in which we plan to add a 400 KeV TEM which will be devoted to these studies. Proposals have been submitted to several Federal agencies for the support of this instrumentation development and a commitment of some University funds to supplement those requested has been obtained.

Our present ion beam facilities utilize a Van de Graaff accelerator which is about twenty years old and is not completely suitable due to its inability to provide heavy ion beams. We plan to upgrade our facility to carry out ion beam analysis by adding a modern moderate energy accelerator capable of using relatively heavy ions. This will enable us to carry out ion beam reaction analysis as well as Rutherford backscattering and channeling measurements.

20. **Please provide a copy of the facility's latest annual report.**

Answer: The Center for the Microanalysis of Materials does not issue a yearly report which is separate from that of the Materials Research Laboratory of which it is a part. A copy of brochure, "Center for the Microanalysis of Materials", is appended.



CENTER FOR

MICROANALYSIS of Materials

UNIVERSITY OF ILLINOIS
AT URBANA-CHAMPAIGN

The University of Illinois has established a Center for Microanalysis of Materials in the Materials Research Laboratory at the Urbana-Champaign campus. The purpose of the center is to house and develop state-of-the-art equipment for the characterization of microchemistry and microstructure in research materials. It is intended that these resources be maintained in the future at the forefront of the field. An excellent technical staff has been assembled for equipment maintenance and development and to assist users in the operation of the equipment for materials research applications.

In cooperation with the Department of Energy (DOE) Materials Sciences Program, it has been planned that this research complex shall be made available to research workers participating in the DOE Universities Program and in the DOE Laboratories Program. Research scientists will be employed by the center to assist users in characterization work needed to accomplish materials research of importance to the DOE mission. In effect the research will be a collaboration between DOE-funded research groups and the scientists at the center. A user interacting with the center will be asked to defray equipment-operating costs through modest usage charges identical with those paid by users located at the Urbana-Champaign campus of the University of Illinois.

The equipment now available to users of the center includes a wide variety of instruments for the analysis of materials' structure and local chemistry with high spatial resolution and high chemical sensitivity. This brochure is made available to inform prospective users about the instrumentation maintained in the center and the type of research results each machine can yield. A listing of personnel responsible for the center is provided on page 16. Prospective users may contact these individuals to discuss use of the equipment.

1

SIMS/Secondary Ion Mass Spectrometry

Two ion microscopes are available for use: a Cameca IMS 3f and an AEI IM20. The Cameca instrument is shown in Figure 1.

Ion microscopes analyze chemical and isotopic composition with a sensitivity that can approach 1 in 10^7 in favorable cases. Space resolution can be better than 1μ on the surface and 50 Å in depth. The instruments operate by means of primary ion beams that sputter secondary ions from the surface into a mass spectrometer. Either a "probe" mode examining a particular spot or an imaging mode providing a real time image of the x-y chemical information can be used for any series of isotopes. In practical cases the sensitivity depends on the resolution required and on the secondary ion yield for the sputtered species. Very large dynamic ranges ($\sim 10^6$) are available. Different primary beams (O, Cs, Ar, · · ·) are employed to optimize the yield for the particular specimen chemistry. High vacuum conditions $\sim 10^{-8}$ torr are maintained in the sample chamber. High and low temperature stages are under development. Constraints on sample geometry are minimal but flat surfaces yield optimal results. Standards are required for quantitative analyses.

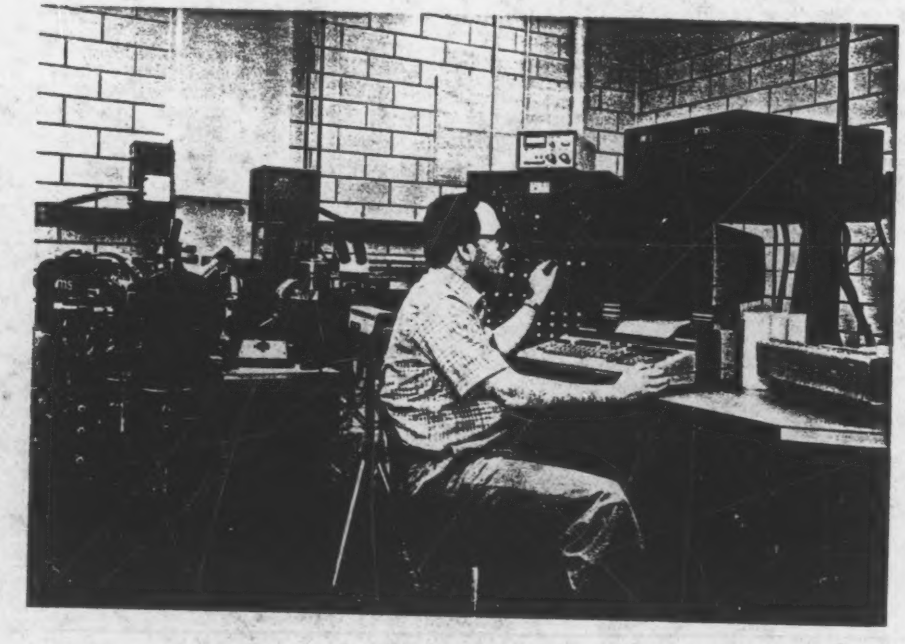


Figure 1

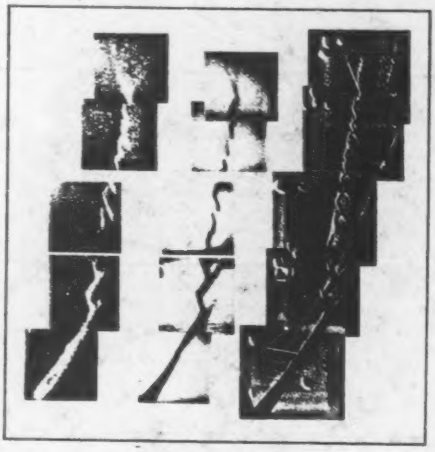


Figure 1a

Cracking of Nb. In Figure 1a the photographs on the left show ion images using the secondary species Nb and NbH⁺ in the neighborhood of a crack tip in fractured hydrogen-embrittled Nb. The photograph on the right is a scanning microscope image of the same crack. The SIMS image identifies excess H on the crack faces. A quantitative determination of H content along the crack yields a concentration close to NbH. Apparently embrittlement arises from hydride precipitation in the stress field of the crack.

Impurity Depth-profiles of as-implanted Be and of the Fe compensating dopant in InP are shown in Figure 1b. The Be and Fe profiles after a 650°C anneal to remove damage are shown in Figure 1c. Both Be and Fe are evidently gettered to the surface and to the damaged subsurface region. Both exhibit anomalous diffusion effects which cannot be predicted theoretically at the present time.

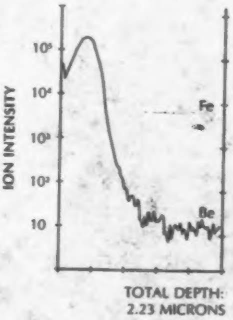


Figure 1b

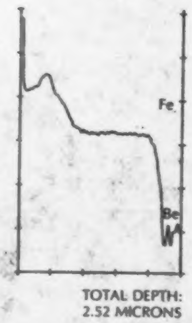


Figure 1c

2

AES/Auger Electron Spectrometry
XPS or ESCA/X-ray Photoelectron Spectrometry

Several major instruments are available for surface chemical analysis. These include the 545 Scanning Auger Microprobe, the 548 ESCA/Auger System, and the 595 Multiprobe, each manufactured by Physical Electronics Industries.

The Auger units detect atomic species in the first few surface monolayers of the sample. The Auger electron emitted from the surface in response to an electron probe beam have energies characteristic of the emitting atomic species; the emission intensities allow the composition in the surface to be determined with a chemical sensitivity of about 0.1 atomic percent. Using the 595 (shown in Figure 2), elemental distribution maps and line scans can be obtained under computer control with an optimal x-y space resolution < 1000 Å. The same electron probe beam allows the 595 to operate as a scanning microscope with resolution of ~ 250 Å. The 545, with 3μ lateral resolution, is available for lower resolution work. Both instruments are equipped with sputter guns for depth profiling purposes.

X-ray photoelectron spectroscopy is available with Auger capabilities at low space resolution in the 548 unit. It can be used to determine core-level shifts caused by the bonding of an atom into its chemical environment and with a chemical sensitivity of about 1 atomic percent.

All this surface-specific instrumentation can operate with the sample in ultrahigh vacuum (10^{-10} torr) and without major constraint on sample geometry. A variety of fracture stages and gas doping capabilities are available.

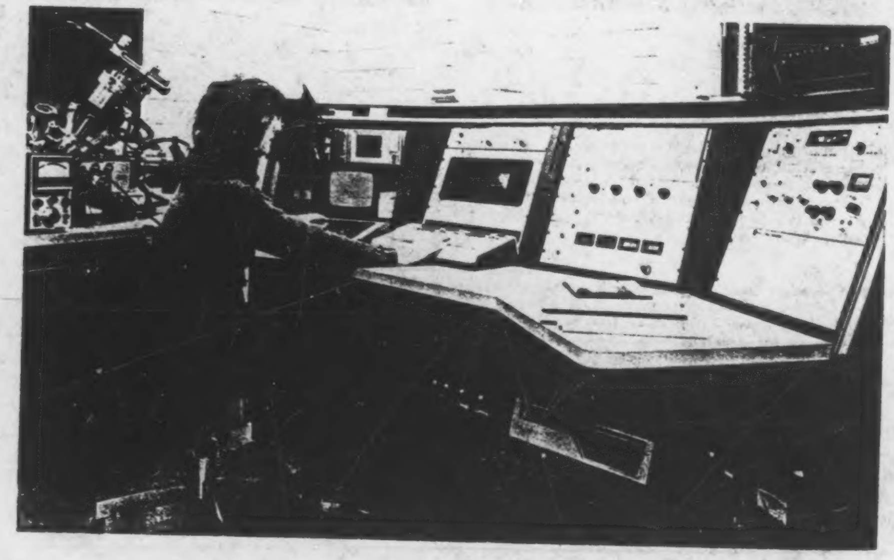


Figure 2

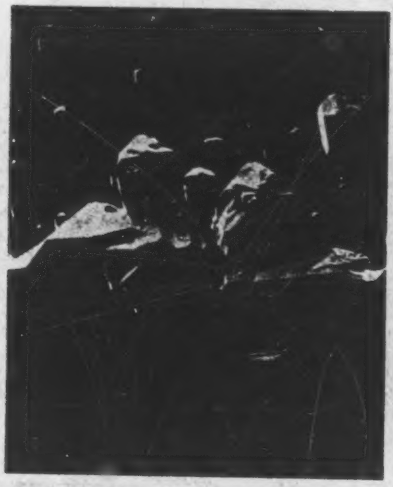


Figure 2a

Figure 2b

Epitaxial Growth of InP. The SEM image from the 595 shown in Figure 2a locates the boundary between good-growth and no-growth regions of an InP film. An Auger spectrum of the no-growth surface reveals C contamination; the C Auger map in Figure 2b identifies C as the source of the growth problem.

Grain Boundary Chemistry. Figure 2c shows Auger line scans for sulfur and chlorine perpendicular to a grain boundary in S doped Ni. The scan detects monolayer-level segregation to the grain boundary.

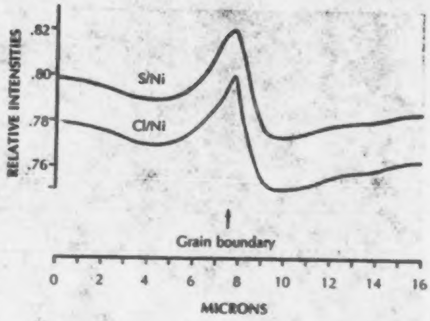


Figure 2c

3

RBS/Rutherford Backscattering
PIXE/Proton Induced X-ray Emission

A Van de Graaf accelerator (Figure 3) is available as a positive ion source operating at about 2 MeV for Rutherford backscattering (RBS) and proton-induced X-ray analysis (PIXE).

In RBS, the He$^+$ beam is directed onto the sample surface and He ions scattered through about 180° are detected by a solid-state, energy-dispersive detector. The kinematic energy loss in the collision can be used to identify the mass of the scattering nucleus (mass resolution is poor above 100 amu) while the inelastic energy loss experienced by the He ions, which can penetrate up to 1 μ before scattering, is proportional to the depth of the scattering center below the surface. Because mass and depth scales are thereby convolved, the technique is most useful for simple thin film systems. Chemical composition can be determined without comparison with standard examples to within 5%, subject to limitations of mass resolution. Depth scales can be determined from tabulated energy-loss data to accuracies of 300 Å. The scattering beamline is being equipped with a conventional vacuum chamber for rapid sample throughput in series with a differentially pumped UHV chamber for clean surface studies.

PIXE analysis involves the detection of ion-induced X-rays generated by MeV protons passing through the sample. The technique is quantitative (about 15% accuracy without standards) and well-suited for repetitive analysis of large numbers of similar samples. Impurity levels as low as 10^{-4} atomic percent can be detected by this method.

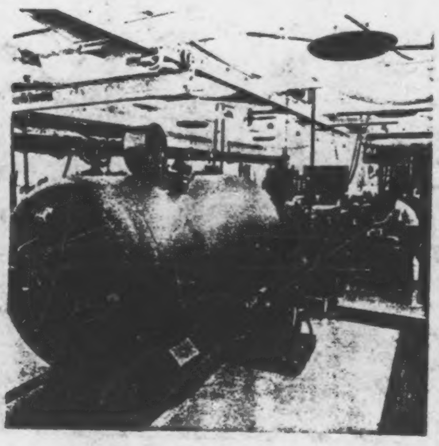


Figure 3

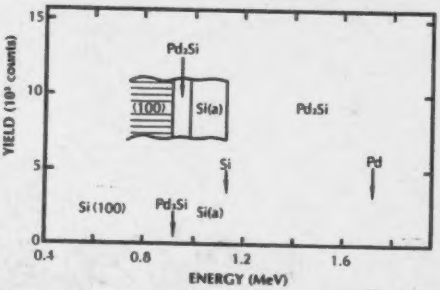


Figure 3a

Analysis of a thin film structure. Figure 3a shows an example of an RBS analysis of a thin film structure: silicon (substrate)/palladium silicide/silicon(evaporated). The Pd spectrum appears at higher energies than the Si spectrum due to the smaller kinematic energy loss of He$^+$ scattering from Pd. He$^+$ scattered from surface Pd would appear at the position indicated by the arrow. The displacement to lower energies of the Pd spectrum shows that the layer is located beneath the surface. A depth scale can be established from published energy-loss tables, and the silicide stoichiometry can be determined from the relative scattering yield from the Si and Pd, corrected for the scattering cross-section (proportional to Z^2). The sample shown here was one of a series of samples in which Pd$_2$Si was used as a diffusion barrier to control solid-phase epitaxy of the deposited Si layer.

STEM/100 kV Scanning Transmission Electron Microscope

The Vacuum Generators HB5 transmission electron microscope (Figure 4) provides an electron beam that may be focussed to 5-10 Å for chemical analysis of small volumes of material. Chemical identification can be made by two methods. X-rays emitted from atoms excited by the beam can be detected and the concentration of the various chemical species determined to about 2% accuracy. The energy lost by the electrons in the beam is also characteristic of the atoms with which the beam interacts, and various species can therefore be detected by means of the spectrum of transmitted electron energies. Energy-loss methods usually work best for light atoms ($Z < 14$) and the X-ray method for heavy atoms ($Z > 12$). Spatial resolution in X-ray analysis is limited by the spread of the beam as it traverses the sample (typically ~ 100 Å for a 1000 Å sample, dependent on sample chemistry). In the energy-loss mode the spatial resolution can be reduced to dimensions comparable to that of the focused beam (~ 10 Å). A new highly efficient spectrometer has been developed at the center to make this method of analysis widely applicable. Ultrahigh vacuum of 10^{-9} torr can be maintained to minimize sample contamination. Electron diffraction can be used to identify the structure(s) in the material through which the beam passes. Microstructures can be imaged with point to point resolution of 3 Å. Specimens must be thinned to about 1000 Å if full advantage is to be taken of this instrument.

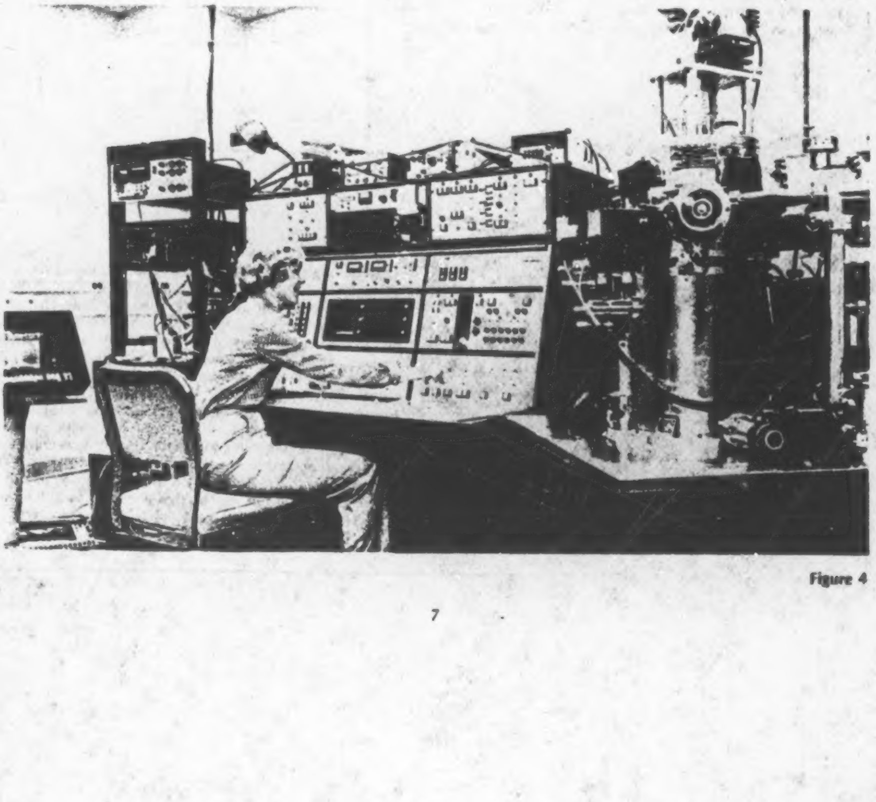


Figure 4

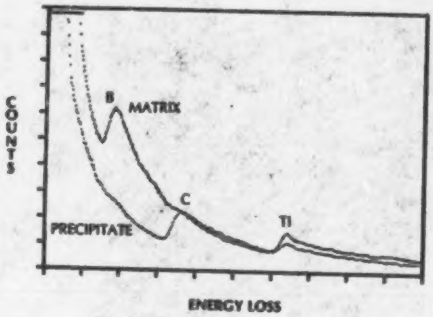


Figure 4a

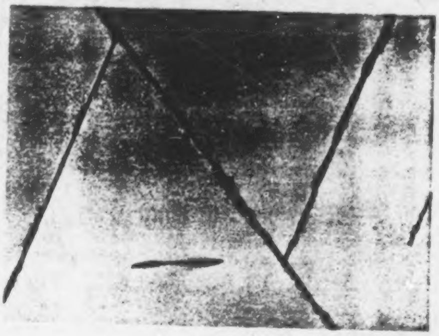


Figure 4b

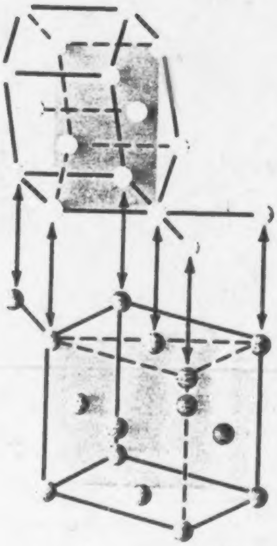


Figure 4c

TiC Precipitates in TiB_2. Figure 4a shows the electron energy-loss spectra for different regions of a TiB_2 specimen in which TiC forms needlelike precipitates (Figure 4b). With a precipitate of the width of < 50 Å, the presence of C and the absence of B is clearly established. Electron diffraction investigations reveal the way the TiC lattice exists coherently in the TiB_2 matrix (Figure 4c). The average C content of the material is less than 10^{-4} atomic percent.

Solidification of a Ti-8Al-4Y alloy. Figure 4d shows an area of the alloy matrix in the as-cast condition. The dislocations making up a subgrain boundary are imaged. At higher magnifications, small precipitates are visible (see Figure 4e). An indication of their elemental composition is given in Figure 4f where it is evident that the second phase is relatively rich in Y.

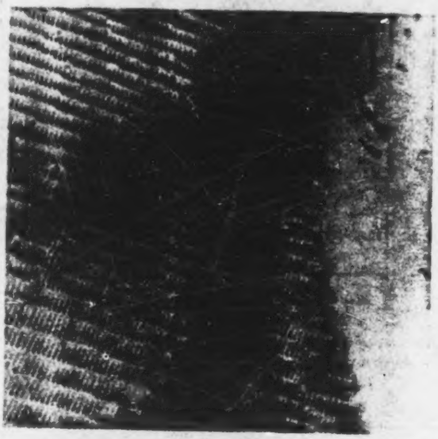


Figure 4d

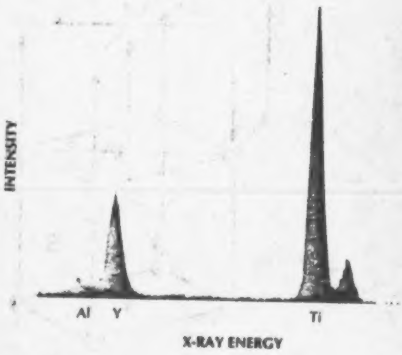


Figure 4f

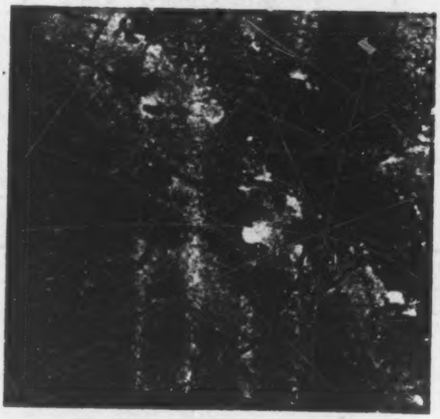


Figure 4e

5

TEM/Transmission Electron Microscope

A Philips EM 400T transmission electron microscope is maintained in the center (Figure 5). Electron diffraction investigations of crystal structure and microstructure are the primary applications of this instrument. Diffraction patterns can be obtained from very small areas of the specimen when the microscope is operated in the convergent beam mode. By means of convergent beam diffraction, it is possible to identify, in an efficient manner, the full three dimensional space group of the material under examination. Analysis can be performed on much smaller sample volumes than those required by X-ray or neutron diffraction methods. The 400T is equipped with a scanning attachment providing a spatial resolution of 20 Å. In the lattice-imaging mode the microscope creates lattice fringe images which reveal the lattice plane structure of the crystal down to a planar separation of 2 Å. Specimens must be thinned to a few thousand Angstroms for effective operation. A variety of specimen stages are available or are being acquired for this instrument.

Since publication of this brochure, we have added a Phillips 420 and 430 TEM to the facility. The 420 is installed and we are awaiting delivery of the 430.

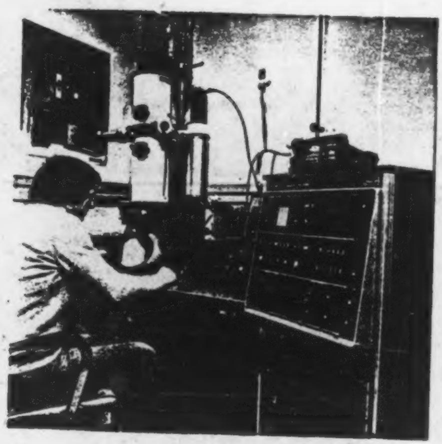


Figure 5

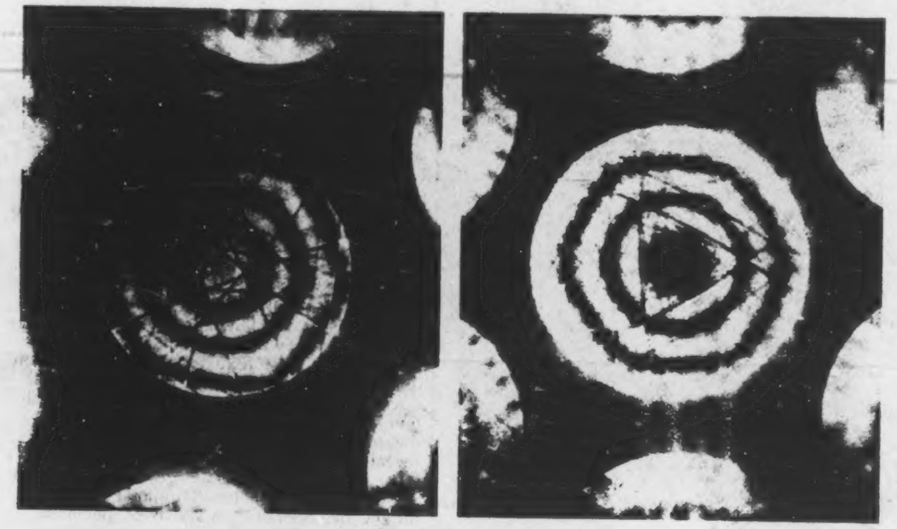


Figure 5a

Figure 5b

Convergent beam electron diffraction patterns for silicon illustrate the variation of the pattern with beam energy. (Figure 5a, left, is 100 kV and right, 120 kV.) The three-fold symmetry of silicon when viewed along a 111 direction is apparent.

Lattice fringes and moiré patterns in a particle of Al_7Cu_2Fe with manganese in Al-2024 alloy are shown in Figure 5b. The sample was rheocast and aged for ten hours at 505°C. The lattice fringes correspond to the (001) plane of the tetragonal structure (c = 1.487 mm). The moiré patterns result from double diffraction in domains having slightly different lattice parameters (1 – 4%) due to the presence of varying amounts of Mn.

6

Workhorse Electron Microscopes and Electron Probes

Additional electron microscopes maintained in the center provide for a variety of general purpose applications. These are the 200 keV JEOL JSEM-200 STEM and two JEOL scanning microscopes, models JSM-35C (Figure 6) and JSM-U3. The 200 keV STEM offers improved beam penetration over 100 keV models and is equipped with X-ray capability for microchemistry. The 35C also has X-ray analysis accessories with computer-based data reduction; in the SEM this provides chemical identification of elements with $Z > 11$ at a spatial resolution of 1 μ. Secondary electrons are imaged with a lateral resolution of 70 Å. Channelling patterns may be obtained from areas as small as 10 μ. The U3 scanning microscope has coarser spatial resolution (~ 200 Å) with a variety of useful specimen stages including a Kossel camera and hot stage.

Also available on campus is a JEOL JXA-50A scanning electron probe X-ray micro-analyzer fitted with two wavelength dispersive spectrometers, each with two crystals, and capable of detecting elements from boron to uranium and an energy dispersive Si(Li) detector. Arrangements can be made for using this instrument through the center. It is a quantitative analytical tool capable in most cases of providing compositions accurate to better than 2% of the absolute value and to a precision approaching 0.1%. The lateral resolution is 1 μ. Data acquisition and sample positioning can be organized by a computer-controlled automated system.

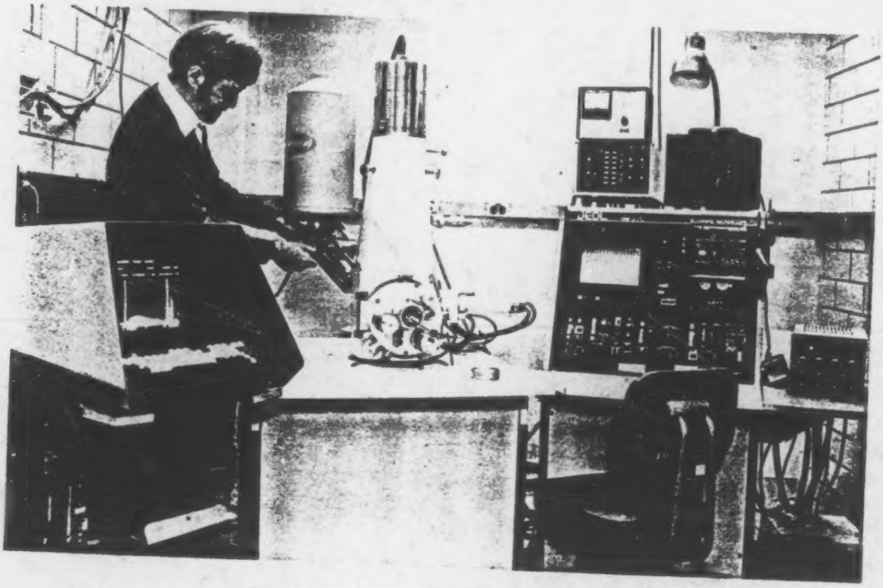
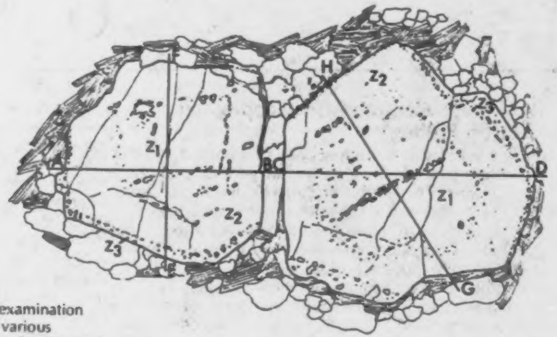


Figure 6



Microchemistry in natural garnets. Figure 6a shows the use of an electron microprobe for examination of the distribution of elemental oxides across various directions in natural garnets. The sketch shows the principal mineral features in outline and the lines along which the concentrations were determined. The distribution of the oxides of Ca, Mg, Fe, and Mn are displayed but not those of Al or Si which make up the rest of the material and whose concentrations are essentially constant over all the garnet.

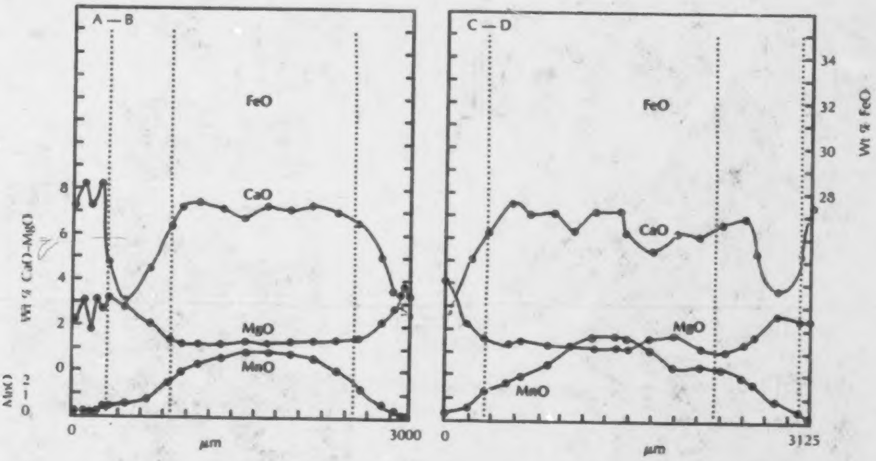


Figure 6a

7

X-ray Instruments

A complex of instruments for X-ray analysis has been established in the center both for materials structure research and for more routine specimen characterization purposes. Two rotating anode sources providing high intensities have been instrumented with four principal beamlines for specialized applications, and a variety of auxilliary systems is available.

Four Circle Diffractometer System. A Huber four circle diffractometer has been set up with an incident-beam, curved-graphite monochromator (Figure 7). The system is fully automated for acquisition and processing of data under computer control. An Elliot GX-21 15 kw rotating anode system operating in the point focus configuration is the X-ray source for the spectrometer. Cu and Mo anodes are available.

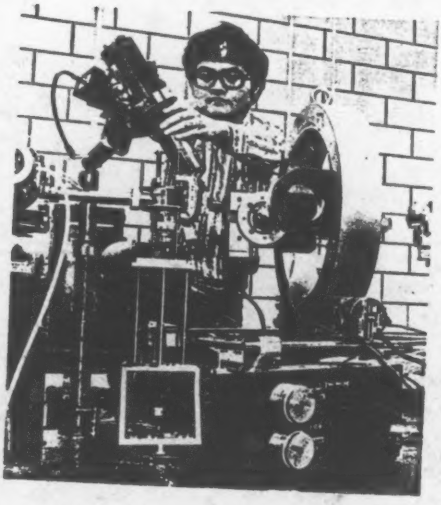


Figure 7

Low Angle Scattering System. A second beamline of the Elliot source is dedicated to a 20-foot-long, small-angle scattering system equipped with a linear multi-ionic detector. The design resolution of the small angle scattering system is 0.01°.

High Resolution Diffractometer System. For measuring lattice parameters and structure modulations with precision, a high resolution X-ray system has been developed with a 12 kw Rigaku rotating anode X-ray generator as the source. The system is computer controlled. It consists of a high resolution triple axis spectrometer with monochromators for the incident and diffracted beams. Either the dispersive +1/+1 mode of the nondispersive +1/−1 mode may be chosen.

EXAFS System. A second beamline of the Rigaku source is dedicated to investigations of local structure in materials through extended X-ray fine structure measurements. Monochromatized X-rays from the Rigaku source pass through the sample, and the fine structure near the X-ray absorption edge is determined from the ratio of the transmitted and incident beam intensities.

Other X-ray Systems. A variety of additional X-ray systems is maintained in the center. These include:

- Picker powder diffractometer with a Debye Scherrer camera using various anode targets,
- Laue transmission and backscattering camera,
- Vertical Philips powder diffractometer with diffracted beam-curved graphite monochromator,
- Automated Kratky small angle camera,
- Burger precession camera with LiF monochromator,
- Weissenberg camera,
- Two Lang topographic camera, and
- Asymmetrical crystal topography system.

Other Services Available to Users of the Center

As far as possible, personnel from laboratories off campus using the University of Illinois Center for Microanalysis of Materials will have access to other central facilities of the Materials Research Laboratory (MRL). The MRL stockroom sells a wide variety of electronic, mechanical, cryogenic, and general laboratory supplies, including metal stock. A ten-man machine shop operated by the MRL is available for emergency repairs of auxiliary equipment belonging to users. The MRL DEC 20-60 computer, operating with 13 time-sharing terminals and two batch streams, is also available to center users. Electron or proton irradiation of materials, cryogenic liquids as needed, mechanical testing, and optical and spark source mass spectroscopic equipment for bulk analysis can be available with sufficient prior notice.

Of particular value to off-campus users may be equipment for specimen spark cutting and thinning, for the preparation of thin film standard samples, for thin film chemical analysis, specimen surface profiling, and so forth. These facilities are available to off-campus users when the center is given advance notice of the need.

Prospective users should contact John Stanley at (217) 333-1372 to arrange beforehand the mechanism for payment of center usage charges and other MRL facility or materials charges. Charges made to off-campus users for research supported by the government are identical with charges made to members of the University of Illinois Materials Research Laboratory.

The Materials Research Laboratory will be pleased to arrange accommodations for users of the center. For assistance in this connection, please call Diana Dougherty at (217) 333-1371.

Center for Microanalysis of Materials

Permanent Staff

J. E. Baker	secondary ion mass spectroscopy
E. G. Boden	electron microscopy
B. E. Clymer	accelerator
I. Dümler	electron microscopy
J. A. Eades	scientific coordinator and instrument development
N. L. Finnegan	Auger spectroscopy
J. A. McMillan	X-ray diffraction
M. E. Mochel	electron microscopy
D. A. Reed	group head: microchemistry
E. A. Sammann	electronics — Auger spectroscopy
F. J. Scheltens	electron microscopy
S. L. Stamer	mass spectroscopy
J. B. Woodhouse	operations coordinator group head: electron microscopy and X-ray diffraction
A. Zangvil	electron microscopy

Operations Committee

H. K. Brinbaum, chairman
J. A. Eades
H. L. Fraser
J. E. Greene
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J. B. Woodhouse
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For information call: J. B. Woodhouse
(217) 333-3888 or 333-0191
D. P. Dougherty
(217) 333-1371

D. Materials Sciences Subprogram

1. What is the detailed budget structure of the Materials Sciences subprogram? What types of work are funded by each of these budget categories?

Answer: The Materials Sciences budget is broken down into funds for operating expenses, capital equipment and construction. General plant projects (GPP), Accelerator and Reactor Improvement and Modification projects (ARIM), and line-item projects are included under construction. Operating expenses are broken down into three categories which reflect the major disciplines utilized in the program - Metallurgy and Ceramics (01), Solid State Physics (02) and Materials Chemistry (03).

In the (01) metallurgy and ceramics category, research is conducted on the structure of materials, mechanical properties, physical properties, radiation effects and engineering materials by metallurgists and ceramists. The principal aim is to understand the relationship between processing, structure and properties. In this category, researchers study for example, the microstructure of dual phase steels, fatigue properties of alloys, oxygen diffusion in ceramic oxides, ion irradiation simulation of swelling of stainless steel, and the effect of welding parameters on weld structure and properties.

In the (02) solid state physics category, solid state physicists study the fundamental properties and theory of the condensed state of matter in the areas of neutron scattering, experimental and theoretical solid state physics, particle-solid interactions and engineering physics. Researchers in this category study, for example, the magnetic structure of rare earth compounds using neutron beams, ion implantation and laser annealing, the electronic structure of surface atom layers in elemental catalysts using synchrotron radiation, the theoretical simulation of crystal defects, ion backscattering to understand the fundamental solidification process, and the use of superconducting devices to map magnetic fields.

In the (03) materials chemistry category, chemical structure, high temperature and surface chemistry and engineering chemistry is studied by materials chemists. The objective is to understand the chemical aspects of materials. Researchers in this category study, for example, the chemical structure of one-dimensional organic conductors, the chemical composition of particle surfaces using infra-red spectroscopy, and the use of laser light scattering to understand surface chemical effects such as corrosion.

Further information on these budget categories and types of research within them is contained in the annual Materials Sciences Program summary booklet, the most recent being the FY 1983, booklet (DOE/ER- 0143/1). The summary report for this subprogram has been published annually since the early 1960's and has received wide circulation, being announced in technical journals, and is the only complete document of its kind in the Federal Government materials research area. This indexed reference document has been of value to both researchers and administrators interested in the content of the Materials Sciences program.

2. For the period FY 1981 - FY 1985, please provide operating expenses, capital equipment, and construction funding for each budget category identified in question 1.

Answer: The funding by year for the Materials Sciences subprogram:

Operating	(M$) FY 1981	FY 1982	FY 1983	FY 1984	FY1985
Metallurgy and Ceramics (01)	38.93	41.07	43.70	48.82	53.27
Solid State Physics (02)	38.21	42.69	53.40	62.91	73.42
Materials Chemistry (03)	11.94	11.75	11.06	13.38	14.79
Total Materials Sciences	89.08	95.51	108.16	125.11	141.48
Equipment*	7.10	7.96	8.51	12.78	15.45
Construction*	0.30	0.60	3.00	16.44	31.72

* Equipment and Construction funds are not allocated by budget category below the subprogram level.

3. For the period FY 1981 - FY 1985, please identify, by budget category and by facility, that portion of Materials Sciences funding going for the support of facilities, such as the National Synchrotron Light Source, etc.

Answer: The following shows the operating funding for the support of the user facilities at each laboratory:

B/A
($ In Thousands)
Operating Expenses

	Budget Category	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
LBL						
NCEM	(01)	600	750	880	1090	1490
ANL						
HVEM/Tandem	(01)	550	600	645	685	750
IPNS	(01,02,03)	3600	3900	3895	4712	5066
BNL						
NSLS	(02)	2800	4500	6172	7962	9400
HFBR	(02)	1472	1900	5996	7033	8800
ORNL						
SHaRE	(01)	200	240	260	290	320
Neutron Scattering	(02)	885	985	275	320	595
Surface Modification	(02)	300	400	485	500	835

	Budget Category	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
LANL						
SNR	(02)	0	0	0	0	500

Note: When allocating capital equipment funds to laboratories, the needs of facilities are considered but not specified below the subprogram level.

4. For the period FY 1981 - FY 1985, please provide, by budget category and by DOE laboratory, the amount of Materials Sciences funding going to DOE laboratories.

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
MATERIALS SCIENCES

(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC02 MATERIALS SCIENCES					
KC0201 METALLURGY AND CERAMICS					
OPERATING EXPENSES					
AMES LAB	$ 2550	$ 2630	$ 2830	$ 3000	$ 3120
ARGONNE NATIONAL LAB	7190	8110	8020	7960	8440
BROOKHAVEN NATIONAL LAB	1760	1740	1850	1960	2080
IDAHO NATIONAL ENG LAB	350	370	400	550	580
LAWRENCE BERKELEY LAB	3330	4190	4630	6120	7070
LAWRENCE LIVERMORE NAT LAB	300	400	674	750	800
LOS ALAMOS NATIONAL LAB	970	990	1197	1370	1460
MOUND LABORATORY	250	120	0	0	0
OAK RIDGE NATIONAL LAB	5500	5811	6272	6780	7150
PACIFIC NORTHWEST LABS	1540	1590	1700	1780	1790
SANDIA CORP	1250	1300	1420	1700	1910
SANDIA LAB, LIVERMORE	400	490	700	750	810
SERI	260	270	290	290	310
KC0202 SOLID STATE PHYSICS					
OPERATING EXPENSES					
AMES LAB	1990	2620	2790	2910	3080
ARGONNE NATIONAL LAB	6060	6038	8140	9130	9680
BROOKHAVEN NATIONAL LAB	8980	12370	18330	20810	23820
LAWRENCE BERKELEY LAB	970	990	1750	4410	5080
LAWRENCE LIVERMORE NAT LAB	720	690	730	770	970
LOS ALAMOS NATIONAL LAB	1390	1780	2300	2290	2780
OAK RIDGE NATIONAL LAB	8290	10220	10066	11330	12950

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
PACIFIC NORTHWEST LABS	340	290	260	270	280
SANDIA CORP	888	960	940	1010	1050
SANDIA LAB, LIVERMORE	100	110	210	230	240
SERI	0	0	60	130	140
KC0203 MATERIALS CHEMISTRY					
OPERATING EXPENSES					
AMES LAB	1470	1470	1540	1610	1700
ARGONNE NATIONAL LAB	4070	4250	3830	3910	4140
IDAHO NTL ENGNG LAB	120	0	0	0	0
LAWRENCE BERKELEY LAB	1280	1310	1420	2770	3150
LAWRENCE LIVERMORE NAT LAB	170	170	180	0	0
LOS ALAMOS NATIONAL LAB	290	310	230	240	260
OAK RIDGE NATIONAL LAB	2580	2755	2700	2920	3100
SANDIA CORP	0	0	0	410	440
KC0281 CHANGE IN INVENTORIES					
OPERATING EXPENSES					
BROOKHAVEN NATIONAL LAB	340	358	550	600	1700
OAK RIDGE NATIONAL LAB	0	- 258	0	0	0
35KC02 MATERIALS SCIENCES					
CAPITAL EQUIPMENT					
AMES LAB	730	730	810	750	800
ARGONNE NATIONAL LAB	1640	1480	1670	2220	2700
BROOKHAVEN NATIONAL LAB	1540	1950	1900	1240	1800
IDAHO NATIONAL ENG LAB	60	30	40	170	60
LAWRENCE BERKELEY LAB	540	660	790	2670	2200
LAWRENCE LIVERMORE NAT LAB	90	50	100	150	200
LOS ALAMOS NATIONAL LAB	300	350	600	900	800
MOUND LABORATORY	20	0	0	0	0
OAK RIDGE NATIONAL LAB	1710	2100	2090	2700	2900
PACIFIC NORTHWEST LABS	170	170	180	200	250
SANDIA CORP	180	220	200	290	340
SANDIA LAB, LIVER	100	200	100	140	150
SERI	20	20	30	50	100
39KC00 MATERIALS SCIENCES					
CONSTRUCTION					
AMES LAB	275	275	275	275	600
ARGONNE NATIONAL LAB	0	0	0	0	0
BROOKHAVEN NATIONAL LAB	350	95	0	3140	11100
LAWRENCE BERKELEY LAB	0	0	0	2060	12290
LOS ALAMOS NATIONAL LAB	0	0	2700	0	0

5. For the period FY 1981 - FY 1985, please provide, by budget category and by institution, the amount of Materials Sciences funding going to universities.

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
MATERIALS SCIENCES

(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
MATERIALS SCIENCES					
KC0201 METALLURGY AND CERAMICS					
OPERATING EXPENSES					
ARIZONA STATE UNIV	$ 0	$ 67	$ 85	$ 94	$ 112
BROWN UNIV	176	201	286	225	340
CALIF UNIV OF DAVIS	145	139	237	223	210
CALIF UNIV OF LOS ANGELES	93	90	61	0	0
CALIFORNIA INST OF TECH	243	241	230	270	290
CARNEGIE MELLON UNIV	53	64	155	75	120
CASE WESTERN RESERVE U	390	259	201	0	178
CATHOLIC UNIV OF AMERICA	57	4	0	0	0
CLARK COLLEGE	0	0	70	0	85
COLORADO SCHOOL MINES	135	145	152	156	185
COLUMBIA UNIV	56	67	79	87	110
CONNECTICUT UNIV OF	195	220	219	70	70
CORNELL UNIV	1062	828	761	1039	805
DARTMOUTH COLLEGE	57	76	88	97	125
DELAWARE UNIV OF	42	44	60	73	80
DENVER UNIV OF	147	77	153	152	160
FLORIDA UNIV OF	90	0	181	105	470
GEORGIA INS OF TECHNOLOGY	60	0	0	0	0
ILLINOIS INST TECH	46	0	- 2	0	0
ILLINOIS UNIV OF	1470	1856	1828	1962	2215
KENTUCKY UNIV OF	69	73	89	71	110
LEHIGH UNIV	205	154	314	76	397
MASSACHUSETTS INST TECH	1372	1521	1613	1396	1912
MASSACHUSETTS UNIV OF	47	28	39	70	0
MICHIGAN STATE UNIV	55	54	61	61	0
MICHIGAN TECH UNIV	75	118	0	94	105
MICHIGAN UNIV OF	62	164	79	176	215
MINNESOTA UNIV OF	1018	964	1029	1406	1100
MISSOURI UNIV OF	128	145	152	116	0
NEW MEX INST MING TECHNL	58	90	95	0	0
NEW MEXICO UNIV OF	0	0	95	0	0
NEW YORK CITY U	56	60	42	0	0
NEW YORK ST UNIV OF ST BROOKE	380	360	460	570	820
NORTH CAROLINA A&T STATE UNIV	0	0	50	0	75
NORTH CAROLINA STATE U	0	10	90	0	110
NORTH CAROLINA UNIV OF	59	38	0	0	0
NORTHWESTERN UNIV	361	211	397	140	230

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
NOTRE DAME UNIV OF	141	0	90	85	75
OAK RIDGE ASSOC UNIV	105	130	140	170	200
OHIO STATE UNIV	200	232	244	370	460
OREGON STATE UNIV	74	50	69	85	90
PENNSYLVANIA STATE UNIV	266	366	396	331	621
PENNSYLVANIA UNIV OF	123	129	139	188	212
PITTSBURGH UNIV OF	61	61	65	71	75
PURDUE UNIV	239	697	760	758	903
RENSSELAER POLYTECHNIC	277	390	291	351	285
RICE WILLIAM MARSH UNIV	0	55	50	55	85
ROCHESTER UNIVERSITY OF	161	172	187	181	95
RUTGERS UNIV	0	51	67	70	90
SERI UNIVERSITY PGM	250	0	0	0	0
SOUTHERN CAL UNIV OF	180	235	251	194	260
SOUTHERN ILL UNIVERSITY	70	73	77	93	100
STANFORD LELAND JR UNVR	386	462	664	589	830
SYRACUSE UNIV	92	80	119	0	180
TENNESSEE UNIV OF	187	134	0	140	0
UTAH UNIV OF	46	57	137	177	289
VIRGINIA POLYTECHNIC INST	113	144	25	77	87
VIRGINIA UNIV OF	0	0	61	0	76
WASHINGTON UNIV OF	66	74	89	92	122
WISCONSIN UNIV OF	36	60	75	90	105

KC0202 SOLID STATE PHYSICS

OPERATING EXPENSES

ARIZONA STATE UNIV	80	98	97	106	120
ARIZONA UNIV OF	0	0	72	75	82
BOSTON UNIV	52	71	162	0	0
BRANDEIS UNIV	0	0	44	0	45
BROWN UNIV	62	59	76	80	89
CALIF UNIV OF IRVINE	191	192	222	214	268
CALIF UNIV OF SAN DIEGO	335	379	399	438	465
CALIF UNIV OF SANTA BARBARA	154	85	244	99	207
CALIFORNIA INST OF TECH	79	75	80	93	97
CARNEGIE MELLON UNIV	69	0	- 7	0	0
CHICAGO UNIV OF	116	118	138	140	157
COLORADO RESEARCH INST	0	0	0	67	71
COLORADO UNIV OF	0	90	187	110	120
CONNECTICUT UNIV OF	0	100	47	80	81
CORNELL UNIV	14	0	0	0	0
DARTMOUTH COLLEGE	106	- 10	0	0	0
DELAWARE UNIV OF	70	81	0	0	0
EMORY UNIV	86	83	44	0	0
FRANKLIN INSTITUTE	0	22	24	25	27
GEORGIA INS OF TECHNOLOGY	115	140	149	159	172
HARVARD UNIV	0	90	365	120	345
HOUSTON UNIV OF	77	74	0	0	0
ILLINOIS UNIV OF	1170	1190	1210	1260	1320
INDIANA UNIV	5	0	0	0	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KENTUCKY UNIV OF	68	71	100	110	105
LOUISIANA STATE UNIV	56	58	62	65	76
MARYLAND UNIV OF	146	155	175	195	210
MASSACHUSETTS INST TECH	159	220	512	317	470
MASSACHUSETTS UNIV OF	43	46	46	35	0
MICHIGAN UNIV OF	64	46	50	75	60
MINNESOTA UNIV OF	213	184	70	115	0
MISSOURI UNIV OF	0	0	175	64	180
NEW YORK CITY U	172	90	85	91	98
NEW YORK ST UNIV OF ALBANY	0	0	5	0	0
NEW YORK ST UNIV OF ST BROOKE	242	399	300	511	550
NORTH CAROLINA STATE U	0	325	275	240	275
NORTHEASTERN UNIV	98	89	79	100	0
NORTHWESTERN UNIV	0	0	110	70	0
OREGON UNIV OF	-32	0	0	0	0
PENNSYLVANIA STATE UNIV	76	47	58	88	75
PENNSYLVANIA UNIV OF	106	110	79	0	94
POLYTECHNIC INST BKLYN	60	65	75	90	95
RENSSELAER POLYTECHNIC	0	110	126	146	120
RICE WILLIAM MARSH UNIV	157	139	180	185	200
RUTGERS UNIV	0	100	122	130	140
SERI UNIVERSITY PGM	250	0	0	0	0
STANFORD LELAND JR UNVR	288	0	0	0	0
STANFORD UNIVERSITY-SSRL	0	0	0	700	1700
STEVENS INST OF TECH	180	65	84	130	104
TEXAS UNIV OF	105	87	90	115	125
VIRGINIA UNIV OF	152	165	176	197	177
WASHINGTON UNIV OF	0	0	70	0	85
WASHINGTON UNIV ST LOUIS	200	0	0	0	0
WISCONSIN UNIV OF	57	61	155	183	174

KC0203 MATERIALS CHEMISTRY

OPERATING EXPENSES

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
CALIFORNIA INST OF TECH	0	0	-8	0	0
CASE WESTERN RESERVE U	-3	0	0	0	0
FLORIDA STATE UNIV	55	56	102	0	0
FLORIDA UNIV OF	110	120	85	0	103
ILLINOIS INST TECH	66	0	0	0	0
JOHNS HOPKINS UNIV	63	70	0	0	0
KENTUCKY UNIV OF	0	94	0	83	86
MASSACHUSETTS INST TECH	75	0	0	0	0
NEVADA UNIV OF	0	0	78	0	0
NEW YORK CITY U - BROOKLYN	0	79	164	90	0
NEW YORK ST UNIV OF ST BROOKE	0	0	90	0	110
NORTHWESTERN UNIV	85	91	0	0	0
PENNSYLVANIA UNIV OF	171	195	154	103	88
PRINCETON UNIV	120	0	73	0	88
RENSSELAER POLYTECHNIC	154	80	89	96	0
STANFORD LELAND JR UNVR	0	0	-2	0	0
TEXAS UNIV OF	0	0	-2	0	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
UTAH UNIV OF	154	163	0	0	0
WASHINGTON UNIV OF	56	151	0	88	94
WEST VIRGINIA UNIV	0	0	57	0	65
WISCONSIN UNIV OF	79	78	83	91	92
KC0281 CHANGE IN INVENTORIES					
OPERATING EXPENSES					
HARVARD UNIV	0	0	8	0	0
35KC02 MATERIALS SCIENCES					
CAPITAL EQUIPMENT					
STANFORD UNIVERSITY-SSRL	0	0	0	100	300
39KC00 MATERIALS SCIENCES					
CONSTRUCTION					
CATHOLIC UNIV OF AMERICA	0	0	0	5000	0
COLUMBIA UNIV	0	0	0	5000	0
NOTRE DAME UNIV OF	0	0	25	25	0
STANFORD UNIVERSITY-SSRL	0	0	0	940	7730

6. **For the period FY 1981 - FY 1985, please provide, by budget category and by company, the amount of Materials Sciences funding going to industry.**

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
MATERIALS SCIENCES

(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC02 MATERIALS SCIENCES					
KC0201 METALLURGY AND CERAMICS					
OPERATING EXPENSES					
BATTELLE COLUMBUS LAB	$ 136	$ 142	$ 114	$ 160	$ 205
BOEING AEROSPACE CO	0	0	75	0	105
FORD MOTOR CO	38	0	0	0	0
GENERAL ELECTRIC CO	70	0	0	0	0
HART FRED ASSOC	0	31	10	0	0
ROCKWELL INTER CORP	196	108	195	140	350

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC0202 SOLID STATE PHYSICS					
OPERATING EXPENSES					
GENERAL ELECTRIC CO	96	0	0	0	0

7. **For the period FY 1981 - FY 1985, please provide, by budget category and by agency, the amount of Materials Sciences funding going to other agencies.**

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
MATERIALS SCIENCES

(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
MATERIALS SCIENCES					
KC0201 METALLURGY AND CERAMICS					
OPERATING EXPENSES					
NAT BUREAU OF STANDARDS	$ 100	$ 80	$ 80	$ 80	$ 80
KC0202 SOLID STATE PHYSICS					
OPERATING EXPENSES					
NAT BUREAU OF STANDARDS	100	80	80	80	80
NAT SCIENCE FOUNDATION	0	0	0	50	0
KC0203 MATERIALS CHEMISTRY					
OPERATING EXPENSES					
NAT BUREAU OF STANDARDS	0	40	40	40	40

8. **How much of the FY 1985 Materials Sciences budget request is for support of programs formerly funded by the DOE Nuclear Program or by any other DOE program?**

Answer: None of the FY 1985 Materials Sciences budget request is for support of programs formerly funded by the DOE Nuclear Program or by any other DOE program.

9. **What have been the major accomplishments of this subprogram over the past five years?**

Answer: Over the past five years, significant progress and accomplishments have been achieved in the areas of: (a) development of new techniques and facilities for preparation, characterization and analysis of materials, (b) understanding of materials phenomena and properties underlying known energy-related problem areas, and (c) discovery of new materials and phenomena which may open new energy-related opportunities for future systems.

The primary purpose of the Materials Sciences subprogram is to increase the understanding of materials phenomena and properties and thereby undergird energy materials development efforts and provide new materials-related options in the long term. This understanding is embodied in the scientific and technical literature containing over 8,000 publications produced by this subprogram in the five-year period. A substantial additional national resource has been the training of over 650 new scientists familiar with materials research of interest to the nation's energy program.

The overriding accomplishment has been the establishment and maintenance of a materials science effort of the highest quality which can be and is being used by the nation's total technical community. This has been done through the appropriate support of forefront materials sciences research in national laboratories, universities, and industry, both through direct support of scientists carrying out the research and through the construction and operation of major facilities necessary for the conduct of materials research by scientists and engineers throughout the nation.

It is well known that materials problems and limitations often impede the performance and feasibility of energy systems as well as other commercially important systems. The following examples of accomplishments have been grouped together to illustrate advances in the development of new facilities, the understanding of certain materials problem areas, and the discovery of new materials-related phenomena which provide options for future exploitation.

a. FACILITIES

During this time period, the formal establishment of 12 collaborative research centers has occurred. This has opened up large, expensive, and special facilities to qualified researchers throughout the nation. The response has been excellent. A recent survey has shown that the centers accommodated about 900 users during a one-year period. The users came from DOE laboratories (21 percent), universities (48 percent), and industry and elsewhere (31 percent). Three of the centers are described in more detail to illustrate the breadth and capability of these facilities.

National Synchrotron Light Source

This facility, dedicated in 1981, is the only dedicated synchrotron source in the world optimally designed to furnish separate VUV and X-ray photons simultaneously. When the facility reaches full design capability it will have the highest brightness characteristics of any existing facility. The VUV ring has operated at 750 MeV and 400 mA and has provided synchrotron radiation to 50 university researchers and 24 industrial researchers since operations began in August 1982. Forefront research on integrated circuits, holography, gas phase spectroscopy, ESCA, and biological structure research is underway. The X-ray ring, not yet fully operational, will operate to 2.5 GeV and 500 mA when it reaches the design characteristics. The intensity and brightness of this X-ray ring will allow a number of forefront areas to be explored. These include X-ray diffraction of micro-samples, powder analysis, topography of dynamical events, surface studies, angiography, and studies of biological molecular structures. It is expected that the number of outside users at NSLS will more than quadruple when the X-ray ring becomes fully operational. Recent accomplishments include the first pictures of the internal structures of living cells with spatial resolution of 0.2 microns, observation of carbon films on niobium which exhibit transitions from amorphous to graphitic to carbide upon annealing, and soft X-rays used to replicate sub-micron integrated circuit features onto photoresist materials. Industrial interest in this area of research has resulted in an investment of more than $5M in beam line instrumentation by such companies as Bell, Exxon, Xerox, and IBM.

Intense Pulsed Neutron Source (IPNS)

This facility, which began operation in 1981, is the first dedicated spallation neutron source for materials science research in the world. As a collaborative research center it has developed into a major source with more than 200 scientists participating in research efforts each year. Although most of the research conducted is related to materials sciences, scientists from other disciplines such as chemists, biologists, and technologists also use the IPNS; these scientists and technolo9ists are from universities, industries and other institutions.

Spallation neutron sources generally have a higher epithermal neutron flux than steady state reactors and therefore complement those facilities in this energy regime. To achieve higher fluxes, important advances have been made on enhanced targets, for example uranium-238, with a success that has resulted in worldwide recognition. Many hundreds of experiments have been performed and a few should be mentioned as representing the unique character of the facility. These include single particle scattering from helium, rapid powder diffraction analysis, non-destructive determination of stress in zircaloy fuel cladding, momentum distributions in the high energy regime, and cryogenic radiation damage studies on a host of magnetic fusion energy materials.

National Center for Electron Microscopy (NCEM)

The National Center for Electron Microscopy at the Lawrence Berkeley Laboratory was dedicated in 1983. The facilities include an atomic resolution microscope for ultrahigh resolution imaging, a 1.5 million electron-volt high voltage electron microscope for dynamic in-situ experiments, analytical electron microscopes for microchemical analyses, and support facilities for specimen preparation, image analysis, image simulation, and instrument development. The instruments will have a major impact on forefront research in metallurgy, ceramics, and life sciences, and are available for collaborative research to qualified users from universities, industry, and other government laboratories. Early results using the high voltage microscope have elucidated the process of defect agglomeration in platinum. The high resolution capability at the center has been exploited to examine grain boundary structure at the atomic level and crystallographic relationships in precipitation phenomena.

b. MATERIALS RESEARCH IN SUPPORT OF ENERGY PROBLEM AREAS (Examples)

Basic research has shown that during the irradiation of alloys, alloying elements interact sufficiently with defects produced by the radiation to cause segregation of the elements. This causes an initially homogeneous alloy to become heterogeneous or, in effect, a composite material. The engineering significance of this phenomenon to nuclear reactor alloy design is pervasive since the microstructure and, concomitantly, properties of the alloys will vary significantly during substantial fractions of their operating lifetimes. Recognition of the importance of this phenomenon to fission and fusion reactor materials development has occurred through numerous workshops, seminars and symposia. The findings of these basic studies have been successfully incorporated into many aspects of reactor materials development, and today they are providing an important underpinning to these materials development efforts.

In other radiation effects research, it has been predicted and discovered that nonenergetic helium atoms form lattice defects in metals and hence nucleate gas bubbles. This understanding alters present thinking on the role displacement-producing radiation plays in helium bubble formation in metals; this must be regarded as a potential problem area in fission and fusion systems. The importance of developing realistic radiation simulation methods has been demonstrated using dual ion beam irradiation to investigate the void swelling behavior of a model stainless steel. To simulate helium gas generation together with atomic displacements, as will occur in a fusion reactor first wall, samples are simultaneously bombarded with helium and heavy metal ions. All aspects of void formation (the kinetics as well as size and spatial distributions) are much different with this method than with the more common technique where helium is preinjected.

Research related to solar energy conversion has led to a number of significant results. Preparation of amorphous silicon by heating silane to 2,300 degrees centigrade with a tungsten source has resulted in the production of high quality material for solar energy conversion. It has been determined that atomic rather than molecular hydrogen is formed, and is responsible for the formation of more perfect bonds in silicon. In other solar related work, a method has been developed to control the di- and tri-hydride content in amorphous silicon hydride. Initial introduction of hydrogen into the amorphous silicon matrix forms silicon monohydride, which has a good photovoltaic response. As more hydrogen is added, however, di- and tri-nydrides form which degrade the photovoltaic properties. Whereas usual single-gap silicon cells have efficiencies in the range of 15 percent, basic research on multigap cells has demonstrated a total solar cell efficiency of 28.5 percent for a cell of aluminum-gallium arsenide in combination with a cell of silicon, i.e , for a two-band-gap solar cell. Simple, yet very high efficiency solar cells have been produced by glow discharge implantation doping of single crystal silicon followed by pulsed laser annealing. The method is easily automated and could radically change the manufacture of solar cells.

In the area of mechanical behavior and corrosion in energy systems, constitutive equations to describe creep deformation of metal alloys (e.g., in high temperature power plant components) have been developed and pioneering work on zircaloy has elicited interest from the electric utilities' Electric Power Research Institute (EPRI). Specifically, EPRI provided material for determining the effects of crystallographic orientation on the behavior of zircaloy-4 fuel pin cladding in light water reactors, so that data needed to assess the validity of constitutive equations for design of reactor fuel pins can be gathered. Deviation from the expected constitutive behavior of zircaloy-4 suggests that a type of defect, grain boundary cavitation, is occurring. This result, confirmed by electron microscopy, helps explain premature cladding failures during power ramping of the reactors and offers guidance to future alloy development. It is known that high hydrogen pressures cause detrimental methane bubble formation in steels. In extreme cases this methanization has caused failure of pressure vessels in petrochemical plants similar to those planned for coal liquefaction. A model has been derived which shows the physical mechanisms controlling various states of bubble growth. An important practical implication of this work is that the bubbles can be removed by proper heat treatment. A common problem in welding stainless steel (used in many energy systems) is cracking at high temperatures. A study of the weld structure after various welding procedures has shown how the structure can be modified so that it is less susceptible to cracking. New research results on stress corrosion cracking (SCC) of alloys in aqueous solutions have shown the importance of borate ions (a threshold ratio of borate to thiosulfate ion) in inhibiting SCC. These results have provided guidance to the evaluation of intergranular SCC of nickel-base alloys in the Three-Mile-Island Unit 1 steam generator.

Analytical electron microscopy has been used to study the effectiveness of certain processing methods for preparing "synthetic rocks" that might provide stable hosts for radioactive waste storage. In one sample (SYNROC-A), an undesirable formation of a thin glass film separating the crystalline phases was detected. This film is undesirable because of its poor leaching resistance. The resultant structural information on these phases is being used to improve the processing methods. A study of simulated radioactive waste glass forms using uranium to substitute for transuranic elements has shown that they do not provide a reliable simulation of the structure and bonding properties of transuranics in silicate glasses. Since the leaching properties are dependent on bonding, this result indicates real waste systems must be investigated for reliable prediction.

In the area of embrittlement of materials, the preference of impurities to segregate to grain boundaries of different orientations has been established for the first time for the case of sulfur and oxygen in iron. This detailed information is a prerequisite for designing alloys with increased resistance to embrittlement. Other research has shown that cesium implanted into nickel binds strongly with hydrogen suggesting the use of cesium to prevent hydrogen embrittlement in critical components. Studies of steels have shown that brittle grain boundaries control fracture at low temperatures, and based on this effective alloy modifications and thermomechanical treatments have been used to inhibit this fracture mode. This may pave the way to future development of nickel-free alloys for use at low temperatures.

In the area of ceramic materials, a new method has been developed for the homogeneous addition of sintering additives to silicon nitride and a procedure derived to prevent the agglomeration of colloidal-sized powder. Homogeneity and retention of colloidal particle sizes are essential requirements to obtain reliable sintered silicon nitride components for systems such as ceramic engines. Fast ion conduction studies in lithium beta alumina by Raman scattering and model calculations have revealed that high conductivity results from correlated motions of ion pairs which indirectly move lithium ions into the conducting plane. These results are important for advances in the area of solid electrolytes in energy systems. In long-term elevated temperature tests, conditions have been identified under which a primary crack will grow based on its interactions with other smaller cracks and cavities in silicon nitride structures. This knowledge will provide guidance on acceptable flaw and phase distributions in high temperature structural ceramics and thus aid in developing realistic design criteria for high temperature energy system components such as large steam turbines or advanced gas turbines.

Research on ion implantation and laser annealing has resulted in a number of important findings. It has been demonstrated that the structure and surface hardness of ceramic surfaces can be modified and controlled by means of post-implantation thermal annealing. On other research, friction has been found to be greatly reduced at iron surfaces as a result of implanting with titanium and carbon ions. An amorphous ternary layer has been observed to form from the process. Materials with improved solar photovoltaic efficiencies have been synthesized. For example, single crystals of silicon implanted with arsenic and annealed with single laser pulses exhibit conversion efficiencies of 15.1 percent. Much cheaper polycrystalline silicon samples exhibit an efficiency of 12.1 percent, which is good for polycrystalline materials. This result is obtained primarily because of impurity profile control by laser annealing.

C. NEW PHENOMENA AND MATERIALS (Examples)

Several areas of theoretical research in the materials sciences have advanced through new insight and through the use of high-speed computers. In the area of electronic structure, computer modeling has successfully predicted the electronic band structure of an elemental semiconductor based only on values of the physical constants. In a similar investigation, the electronic band structure of complex ternary photovoltaic compounds has been calculated. Both of these modeling techniques have the potential to predict how to tailor materials for optimum photovoltaic properties. A new phenomenon of magnetic field shielding that would reduce stray magnetic fields to the microgauss level has been calculated for a cylindrical superconducting device. the concept has been patented and has potential impact on supercomputer development as well as on greatly increasing the sensitivity for micromagnetic detection and measurement. The difficult area of glassy solids has been successfully probed through computer simulation of the new phenomenon known as "quench-echoes" in these random materials. This result is important to understanding low-frequency excitations in glasses, which is an advancing field. Several theoretical studies of ultrarapid solidification processes are underway to understand the phenomenon of homogeneous bulk nucleation resulting from short-burst laser pulses on materials. In the case of silicon, it has been shown and experimentally confirmed that bulk nucleation occurs during the laser pulse and determines the maximum penetration of the melt front. This information resolved a major controversy regarding the mechanism of energy absorption by materials and is important for all rapid solidification processes.

Amorphous or metallic glasses were discovered under a Materials Sciences contract and are now being developed for a number of applications including electrical transformer cores where their extremely low hysteresis loss may result in annual savings of 300 million dollars. Since these materials are normally produced by rapidly quenching liquid streams into thin solid ribbons, applications have been limited to those where ribbons can be used, in spite of the fact that the materials themselves possess significantly enhanced corrosion, mechanical and other properties over many normal crystalline materials. Follow-up investigations have recently shown that metallic glasses can be prepared at low temperatures without quenching by directly reacting crystalline materials with certain rapidly diffusing species. This discovery has at least two significant implications. First, from a scientific point of view, the discovery that equilibrium crystalline materials can be made to transform spontaneously to nonequilibrium amorphous materials is exciting. Second, this discovery portends the possibility of preparing bulk (as opposed to thin ribbons) metallic glasses, thereby making metallic glasses with their enhanced properties accessible to a wider range of applications.

Until 1980 it was firmly believed that ferromagnetism and superconductivity, two forms of order in materials at low temperatures, were incompatible; that is, they could not coexist in the same material according to the prevalent theories of the day. However, measurements made in the mid-1970s of two unusual ternary compounds, erbium rhodium boride, and holmium molybdenum sulfide, suggested evidence for the existence of magnetism and superconductivity at temperatures below one Kelvin. In the early 1980s there was considerable research activity to determine the nature and interactions of the magnetism and the superconductivity in these two and other related compounds. Using neutron scattering it was found that for a small temperature range, ferromagnetism and superconductivity coexist in erbium rhodium boride. These and other new observations have contradicted the theories of the day and have given rise to improved theoretical understanding of both superconductivity and ferromagnetism.

Research on metallic alloys and compounds has resulted in a number of significant accomplishments Unique electron microscopy facilities have made it possible to optimize the structure of steel for strength, fracture resistance and fabricability. As a result, a new class of dual phase steel alloys having greater strength and fracture resistance per unit weight and which can be fabricated using current commercial methods has been developed. The annual energy savings possible through weight reduction by using these dual-phase steels in cars, trucks, and trains may approach 10 percent of the quads currently consumed by the transportation sector.

A new in-situ process has been developed for preparing multifilamentary superconducting wire at significantly reduced cost. Superconducting wire is used in magnets for NMR imaging, fusion energy research, and high energy physics and it has potential for use in power transmission and generation equipment. A class of materials called intermetallic compounds, such as Ni_3Al, which have excellent high temperature strength and corrosion resistance has been successfully fabricated by understanding principles of alloy thermodynamics and high temperature deformation. Heretofore, their use has been limited because of brittleness which has now been significantly reduced. Research with niobium and tantalum covered with a few atomic layers of palladium has resulted in the discovery that hydrogen is absorbed at greatly increased rates compared with single atomic layer coverages or no palladium coverages at all. This discovery may assist efforts in large scale storage of hydrogen for energy systems.

Research on the synthesis of materials by deposition has resulted in a number of new materials. Using chemical vapor deposition (CVD), a hard, wear resistant coating of titanium diboride has been produced which shows promise for use in valves in coal liquefaction. The technique developed is capable of depositing adherent, porous-free titanium diboride which exhibits excellent erosion resistance. Also using CVD, an important, new high-temperature solar-absorbing film has been synthesized. The material, zirconium diboride, shows excellent long-term stability in air at 600°C. Using electric-field-induced sputtering, fabrication of complex ceramic coatings has been shown possible by understanding the relationship between sputter parameters and microstructure. This understanding has permitted the formation of coatings containing controlled chemical composition (graded from metallic to ceramic at the outer edge) and structures that are capable of withstanding severe thermal cycling. Low energy deposition of very low concentrations of platinum on surfaces of titanium (about one atom in a thousand) has resulted in two dimensional arrays of platinum possessing high surface areas and enhanced catalytic activity; this offers potential guidance for designing low-cost catalysts.

Research on materials characterization and instrumentation has led to a number of significant developments. Two triple-axis superconducting quantum interference devices (SQUID), devices capable of measuring minute changes in the earth's magnetic field, have been successfully deployed 4.8 kilometers apart near the San Andreas Fault in California. With this ultra-sensitive apparatus, long-term monitoring of the earthquake zone can take place and the onset of earthquakes may be predicted. Developments in new sophisticated instrumentation with SQUIDs have resulted in devices that operate at temperatures of about 16K, the highest yet reported. These devices are especially sensitive for deep earth geothermal exploration (more than 10 km) at low frequencies (less than 10 Hz). Actual field tests in a known geothermal area have correlated a geological fault line sequence with a known source and have predicted new source areas which will soon be explored for confirmation.

Using radiation from a synchrotron radiation source, the surface structure and temperature distribution for silicon after laser heating were determined for the first time. By combining the probes of small angle neutron and X-ray scattering, the size, shape, and pore distribution of oil contained in oil shale have been determined nondestructively for the first time. These techniques will greatly assist the development of extraction technology as well as enhanced oil recovery schemes.

New diagnostics using photoemission have been applied to battery systems, especially electrolyte solutions, where as little as 2 parts per billion iodine has been detected at the liquid surface. These same studies, which make use of the newly discovered Giant Raman Effect, have identified adsorbates under water; this has not been possible to accomplish with standard spectroscopic techniques such as infrared or electron energy loss spectroscopy.

Neutron "time-of-flight" techniques have been successfully used to measure residual stresses in tungsten carbide cermet materials and in a zirconium alloy. The information on cermet materials is important in the design and development of drilling inserts for oil and gas well drilling apparatus. The detailed information on residual stresses in the zirconium alloy provides valuable data for reactor fuel element and pressure tube design and performance analyses.

Development of a portable infrared detection instrument makes possible real-time rapid airborne study of plume chemistry which will help control acid rain. A real-time airborne analysis above a coal-fired power plant plume has been conducted for the first time and revealed unusual sulfate particle distributions over short-time periods (as little as thirty minutes after leaving the stack) and over considerable distances (tens of miles).

10. For the period FY 1981 - FY 1985, how much funding has this subprogram provided and is estimated to provide for the R&D of experimental devices/apparatus?

Answer: A research program at the frontier of science necessarily must be developing new techniques which involve building or modifying experimental devices or apparatus. It is difficult to estimate what is spent on research and development associated with devices as distinct from research using available devices. Almost every experimental project has some aspect of research and development on experimental devices. The research and development associated with construction projects is very clear and is specifically identified in each construction project data sheet. Other activities related to research on and/or development of experimental devices are diffused throughout the program and can only be estimated, without a questionnaire going out to every investigator. An approximate figure would be about 1-5% of the operating funds plus about 5-10% of the capital equipment.

11. How does the research funded by the Materials Sciences subprogram differ, complement, supplement, or overlap materials research funded by other parts of DOE, as well as by other agencies such as the National Science Foundation and or the Office of Naval Research?

Answer: The research funded by the Materials Sciences subprogram is designed to underpin the Department of Energy needs and requirements in the long term for materials research. It differs substantially in character from the other DOE materials programs in that it fulfills the need for increased understanding of classes of materials, materials phenomena and technique developments of importance to a number of DOE programs. The research is at the fundamental and generic end of the spectrum. Materials research in other DOE programs is aimed at specific systems applications, whether it be nuclear fission, solar energy, fossil energy, etc. The work within the Department is coordinated primarily by means of the Energy Materials Coordinating Committee. Strong interaction between the basic and applied researchers exists at several points, but there is a conscious effort to avoid overlap. To enhance technology transfer, there are cases where the same research group at a laboratory receives funding from the Materials Sciences subprogram as well as from some other DOE applied program. Insofar as interactions with other agencies are concerned, the Materials Sciences subprogram has the responsibility to underpin the research and development objectives of the DOE. DOE is a mission agency, as are the other agencies such as ONR, etc. The National Science Foundation, on the other hand, supports research that has as its objective the furtherance of science. The NSF also tends to support areas which clearly do not fit into any mission agency. Some research areas in materials are clearly of interest to several agencies. In those cases, the agencies coordinate to assure that no overlap is created. In general, the overall thrusts of the different agency programs are divergent and the funds are scarce enough to encourage coordination and present overlap.

12. What types of formal and informal advisory groups does the Division of Materials Sciences employ to assure that the subprogram is of high quality and coordinated with the research carried out at other agencies? If any formal advisory groups exist, please define the role of each, and provide a listing of the current membership.

Answer: The Division of Materials Sciences does not have an overall formal advisory group. Parts of the program such as those at DOE laboratories, have program advisory committees and certain university programs do also. The quality is assured by various review processes and coordination is assured primarily through established coordination committees at the DOE headquarters level. The Council on Materials Science assists the Division in selecting areas of research for emphasis and review. The Council also has undertaken the role of reviewing the research at major facilities.

The process of review takes a number of forms. Unsolicited proposals are peer reviewed. An annual on-site review takes place at each DOE laboratory. An annual proposal review for each DOE laboratory takes place at DOE headquarters. Management arrangements at the DOE laboratories require appropriate peer reviews to be undertaken by the laboratories of their own activities. An annual headquarters competition award process with DOE laboratory participation is aimed at the same objective of assuring quality.

Ad hoc technical reviews of specific research areas are undertaken as needed, and workshops are held to stimulate thinking or expose groups of researchers to one another for the purpose of maintaining frontier programs. Coordination takes place at various levels including individual contacts and exchange of documents among researchers in the usual scientific mode. The Division has compiled an annual listing and index of the programs it supports, since the early 1960's and distributes it widely to other agency personnel and to researchers in the field. In areas of high visibility, a bulletin is published and exchanged among researchers to keep them up to date on the latest findings and plans. Within the Department of Energy, the materials research programs are coordinated in a formal way through the Energy Materials Coordinating Committee and its various sub-committees. An annual technical report is compiled and published. At the Federal agency level, many formal committees exist. The Interagency Committee on Materials coordinates the Programs of the funding agencies for basic materials research. A number of topical committees exist, such as the Interagency Ceramics Committee and the Interagency Intense Photon Source Committee. At the OSTP level, the Committee on Materials (COMAT) assists in coordinating the Federal programs in materials, both basic and applied. COMAT has subcommittees on welding and on rapid solidification technology. The Division of Materials Sciences is an active participant on all these coordinating bodies.

The mechanisms for obtaining information on program emphasis and direction are many and varied. The Council on Materials Science, which consists of scientists from academia, industry and the DOE laboratories was the outgrowth of a series of workshops held in 1976 to help refocus the program in the conversion from an AEC (Atomic Energy Commission) program to a total energy program. The Council has sponsored a number of Panel meetings which are held for the purpose of stimulating ideas in an area deemed to be important for the future. These Panel meetings have resulted in high quality reports published in the open literature to a large extent. In interfacing with the DOE applied programs, a formal mechanism has been established called the Research Assistance Task Force. Where an area of mutual interest has been identified by both the basic research program and the applied program, a meeting is held to bring together researchers from both programs for the purpose of exchanging views and identifying further research to be undertaken. These meetings have been successful in coordinating the basic and applied research within the Department. This is only a brief summary of activities aimed at assuring a high quality well coordinated program.

13. What is the current rate of Ph.D. production in the materials sciences?

Answer: The Ph.D.'s awarded in 1983 to students who have support from the Department of Energy, Materials Sciences Division, is about 180. This includes students from the two DOE laboratories associated with universities, University of California at Berkeley (LBL), and Iowa State University (Ames Laboratory) and those performing their research at the DOE National Laboratories.

14. What is the average cost to produce a Ph.D. in this field?

Answer: The average cost of a Ph.D. in materials sciences is approximately $270,000. The costs range from $150,000 for a theoretical scientist who does not use expensive equipment or facilities to $400,000 for an experimentalist utilizing state-of-the-art facilities and equipment such as synchrotron radiation, or neutron scattering. The costs ranges are derived by dividing the total annual program supported in an area by the number of students receiving a Ph.D.

15. Has the number of materials sciences researchers supported by this subprogram been increasing, stable, or decreasing over the past five years? What change will occur given the FY 1985 budget request?

Answer: The number of materials sciences researchers has decreased about five percent in the period from fiscal year 1980 to 1984. This overall result is the sum of two opposite trends--a significant decrease (in excess of 10 percent) in materials scientists supported at DOE laboratories versus a considerable increase (nearly 10 percent) for university supported scientists. Given the fiscal year 1985 budget request coupled with the costs associated with facilities, an additional small (a few percent) reduction in the number of scientists supported will occur, wholly from the DOE laboratories. Overall the number of principal scientists supported in the subprogram has gone from about 900 in FY 1980 to an expected level of slightly over 800 in FY 1985.

16. What is the average annual cost per year to this subprogram to support a materials sciences researcher?

Answer: In FY 1984 the average annual cost per year per researcher is about $123,500. To obtain this cost, the total number of principal and co-principal investigators is divided into the total operating costs minus the costs associated with the operation of user facilities. If you include capital equipment in the same manner, the average annual cost would be about $137,200.

17. Please provide a copy of the latest Materials Sciences research summaries.

Answer: A copy of Materials Sciences Programs, Fiscal Year 1983, DOE/ER-0143/1 is attached. These summary reports are published annually in the Fall of each year.

1.0 Advanced Synchrotron Radiation Research Planning Study Committee Interim Report

18. In its November 14, 1983 interim report, the Advanced Synchrotron Radiation Research Planning Study Committee recommended as its first priority "expeditious completion of current projects to construct insertion device beamlines at SRC, NSLS and SSRL." What is the Department doing in FY 1984 and expect to do in FY 1985 to address this recommendation?

Answer: The U.S. Department of Energy is not directly responsible for the development of the facilities at SRC since this is an NSF project and DOE has not received any requests for assistance for such development. The wiggler/undulator technology developed under DOE sponsorship elsewhere will of course be available to SRC. Scientists from LBL have assisted SRC in technical matters with DOE concurrence.

FY 1984 operating funds have been allocated to conduct the necessary research and development for the insertion devices and beamlines associated with the construction of NSLS Phase II. This includes three specific multipole wigglers (a hybrid wiggler for high Q-resolution, a soft x-ray wiggler for x-ray microscopy and holography, and a superconducting wiggler for hard x-ray applications such as medical imaging and invasive chemical techniques) for the x-ray ring and also general consideration of undulators and wigglers for the vacuum ultraviolet as well as the x-ray ring. In FY 1985 the Department expects to make available funds to extend this R&D work and to begin construction of these insertion devices at NSLS. These activities and plans are clearly spelled out in the FY 1984 and FY 1985 congressional budget submissions.

The Department's actions in FY 1984 for the expeditious completion of current projects involving insertion devices at SSRL were included in the construction project termed NCAM - which is being reviewed by Congress. FY 1984 operating R&D funds were allocated to support research and development of insertion devices for both SPEAR and the PEP ring - the work is a collaborative effort of SSRL and LBL. FY 1984 construction funds for SSRL when made available will be used for the construction of SPEAR Insertion Device Shielding and the PEP Undulator Beam Line Tunnel and the construction of the associated insertion devices - a 26-period, 2-meter rare-earth cobalt undulator for the PEP ring and a 54-pole rare-earth cobalt wiggler for the SPEAR ring.

For FY 1985 the Department has incorporated a number of the recommendations of the Advanced Synchrotron Radiation Research Planning Study in its request to Congress. For example, the SSRL Enhancement Construction Project has been separated from the LBL CAM project and funding is requested for continuation of this project as well as NSLS-II.

19. As a second priority, the Committee recommended "the construction of a 6 GeV storage ring beginning in 1987 as a dedicated national facility," with "appropriate R&D funds..allocated in FY85 and FY86." What funding is available in the FY 1985 budget request to support this recommendation?

Answer: Research and Development operating funds totaling $3.8 M in FY 1985 for research at LBL are requested for generic photon research activities at LBL but none specifically for a 6 GeV storage ring concept. This generic research on undulator/wigglers and beam line optical components, as examples, is important to the improvement of the research capabilities of current synchrotron radiation sources, such as SSRL and NSLS, and as preconstruction R&D for future advanced photon sources. The 6 GeV synchrotron would be such a source.

20. As its third priority, the Committee recommended "proceeding with the ALS in FY85 as a dedicated national facility." What funding is available in the FY 1985 request to address this recommendation?

Answer: No construction funds in FY 1985 are requested for this purpose. Decisions on constructing ALS will be made after the report of the NAS Committee on Major Materials Facilities has been completed and reviewed. Operating funds of $3.8 million and capital equipment funds of $0.7 million have been requested to conduct generic research and development on future light source problem areas.

21. Finally, the Committee "strongly" recommended "that no action on a lower priority recommendation interfere with the timely pursuit of the higher priority items." Is the Department's FY 1985 request consistent with this recommendation?

Answer: Our FY 1985 request is completely consistent with this recommendation as reflected in our responses to questions 19 and 20.

2.0 Advanced Materials Initiative

22. The Department's FY 1984 request for its Advanced Materials Initiative totalled $38.0 million, including $28.4 million for construction, $7.7 million for operating expenses, and $1.9 million for capital equipment. Only $3 million was appropriated for construction, but the remainder of the operating and capital equipment funds were appropriated. Please describe in detail the distribution of these funds.

Answer: The following describes the distribution of the FY 1984 appropriations associated with the Advanced Materials Initiative:

(Dollars in Thousands)

	Operating		Equip
SSRL	700	(R&D associated with the SSRL construction project)	100
LBL	2300	(Initiation of research programs in ceramics, electronic materials, catalysis and surface instrumentation, and polymers)	1300
BNL	1000	(R&D associated with construction of and in preparation for NSLS Phase II)	

	Operating	Equip
LBL	3200 (R&D on generic problems associated with advanced photon systems, vacuum systems, wigglers and undulators, beam line components as part of the newly formed optics center)	500
Contract Research	500 (For new university research associated with advanced photon systems)	

23. **The Department's FY 1985 request for the Advanced Materials Initiative includes $12.55 million for "Programmatic Research and Research and Development Associated with Construction." Please describe in detail the plans for the use and distribution of these funds.**

Answer: Since the submission of the budget we have determined that the total for equipment plus operating funds for the Advanced Materials Initiative is only $11.52 million. The plans for the use and distribution of the funds called out for programmatic research and research and development associated with construction are:

B/A
$ in thousands

	Operating Funds	Equip. Funds
SSRL	1700 (R&D associated with construction, 700, and materials sciences operations funding at SSRL, 1000)	300
LBL	3800 (Generic R&D on advanced photon systems and beam lines including the optics center research)	700
LBL	2900 (continuation of center for advanced materials research programs on ceramics, catalysis and surface instrumentation, electronic materials, polymers, and an additional effort on alloy deformability)	600
BNL	500 (R&D associated with construction of NSLS Phase II)	
Contract Research	470 (For university research associated with advanced photon systems)	550
Total	9370	2150

24. **The *ad hoc* Technical Review Panel to Review the Lawrence Berkeley Laboratory Proposal for a National Center for Advanced Materials (NCAM) specifically recommended that final judgement of activities in the areas of Advanced Materials Synthesis and Advanced Device Concepts "be delayed until an acceptable NCAM' program plan is available," and that the construction of the Advanced Materials Synthesis Laboratory/Advanced Device Concepts Laboratory (AMSL/ ADCL) facility "be deferred until a subsequent review of that plan has been completed." Furthermore, the Panel questioned "whether organizing materials synthesis as a separate, programmatic activity is wise," and suggested "that LBL consider strengthening the materials-synthesis effort in the MMRD, consistent with NCAM' growth." Given the above, why does the FY 1985 budget request include a request for the initiation of funding of the Advanced Materials Laboratory at LBL?**

Answer: The FY 1985 budget construction request includes $1.6 M for the initiation of funding of the Advanced Materials Laboratory (AML). The AML is essential for the success of the Center for Advanced Materials, and would provide needed equipment and space for the focused advanced materials research program, other than surface science and catalysis. The original idea of having a separate synthesis laboratory has been modified taking into account comments and recommendations of the Panel and others during last year's extensive reviews. The timing of this building is consistent with the review panel's recommendation which stated that the building should await an acceptable CAM program plan. A strong effort was undertaken, since the Panel report was completed to identify topics, receive industry input and to review the plan and building needs. This has been done by LBL and reviewed and approved by DOE. An Advisory Scientific Policy Board has been established, and an Interim Director, Dr. Kenneth Pitzer, a distinguished scientist, has been given responsibility for the evolution of the research program until a permanent Director is named. In view of the progress made to date and the long lead time before the building can be occupied, we believe this request is completely reasonable and essential in order that there be a center for advanced materials research at LBL.

September 1983

Materials Sciences Programs

Fiscal Year 1983

FOREWORD

The Division of Materials Sciences is located within the Department of Energy in the Office of Basic Energy Sciences. The organizational structure of the Department of Energy is given in an accompanying chart. The Office of Basic Energy Sciences reports to the Director of the DOE Office of Energy Research. The Director of this Office is appointed by the President with Senate consent. The Director advises the Secretary on the physical research program; monitors the Department's R&D programs; advises the Secretary on management of the multipurpose laboratories under the jurisdiction of the Department, excluding laboratories that constitute part of the nuclear weapon complex; and advises the Secretary on basic and applied research activities of the Department.

The Materials Sciences Division constitutes one portion of a wide range of research supported by the DOE Office of Basic Energy Sciences. Other programs are administered by the Office's Chemical Sciences, Biological Energy Research, Engineering, Mathematical and Geosciences, Advanced Energy Projects, and Carbon Dioxide Research Divisions. Materials Sciences research is supported primarily at DOE National Laboratories and Universities. The research covers a spectrum of scientific and engineering areas of interest to the Department of Energy and is conducted generally by personnel trained in the disciplines of Solid State Physics, Metallurgy, Ceramics, and Chemistry. The structure of the Division is given in an accompanying chart.

The Materials Sciences Division conducts basic research on materials properties and phenomena important to all energy systems. The aim is to provide the necessary base of materials knowledge required to advance the nation's energy programs.

This report contains a listing of research underway in FY 1983 together with a convenient index to the program. Recent publications from Division-sponsored panel meetings and workshops are listed on the next page.

Louis C. Ianniello, Director
Division of Materials Sciences
Office of Basic Energy Sciences

RECENT DIVISION SPONSORED PUBLICATIONS

Topical and Workshop Reports[a]

- High Pressure Science and Technology (1983)
- Scientific Needs of the Technology of Nuclear Waste Containment (1983)
- Materials Preparation and Characterization Capabilities (1983)
- Critical and Strategic Materials (1983)
- Radiation Effects (1982)
- Condensed Matter Theory and the Role of Computation (1981)
- Research Opportunities in New Energy-Related Materials (1981)[c]
- Aqueous Corrosion Problems in Energy Systems (1981)[c]
- High Temperature Corrosion in Energy Systems (1981)[c]
- Basic Research Needs and Opportunities on Interfaces in Solar Materials (1981)[c]
- Basic Research Needs on High Temperature Ceramics for Energy Applications (1980)[c]
- Organic Conducting Materials[b]
- Coatings and Surface Modifications[b]

Summary Research Bulletins (of Work in Progress)[a]

- Ceramic Processing
- Erosion and Wear
- High Voltage Electron Microscopy
- Non-Destructive Evaluation
- Sulfur Attack
- Welding

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[a] Available in limited quantities from the Division of Materials Sciences.
[b] To be published.
[c] Also published in Materials Science and Engineering.

ORGANIZATION OF THE DEPARTMENT OF ENERGY

Department of Energy

Secretary
Deputy
Under Secretary

Assistant Secretaries

1. Nuclear Energy
2. Defense Programs
3. Environmental Protection, Safety and Emergency Preparedness
4. Conservation & Renewable Energy
5. Fossil Energy
6. International Affairs
7. Management & Administration
8. Congressional, Intergovernmental & Public Affairs

Office of Energy Research

- Federal Energy Regulatory Commission
- Economic Regulatory Administration
- Energy Information Administration

Office of Energy Research

Director
Deputy

Associate Directors

1. Field Operations Management
2. Program Analysis
3. Fusion Energy (Magnetic)
4. High Energy & Nuclear Physics
5. Health & Environmental Research
6. Basic Energy Sciences
    - Materials Sciences
    - Chemical Sciences
    - Engineering, Mathematics & Geosciences
    - Advanced Energy Projects
    - Biological Energy Research
    - Carbon Dioxide Research

- Management
- Special Programs (Small Business Innovation Research)

STRUCTURE OF

DIVISION OF MATERIALS SCIENCES

OFFICE OF BASIC ENERGY SCIENCES

Materials Sciences

Director
L. C. Ianniello
(Sandy Tucker - Secretary)

Metallurgy and Ceramics Branch

(Janet Venneri - Secretary)

Chief: Vacant
S. M. Wolf
R. J. Gottschall
F. V. Nolfi, Jr. 1/
D. M. Parkin 2/

Solid State Physics and Materials Chemistry Branch

(Linda Twenty - Secretary)

Chief: M. C. Wittels
T. A. Kitchens
B. C. Frazer 3/
J. B. Darby, Jr. 4/
M. Weber 5/
H. G. Smith 6/

Notes:
1/ On Leave from Ames Laboratory
2/ Return to Los Alamos National Laboratory 7/83
3/ On Leave from Brookhaven National Laboratory
4/ Return to Argonne National Laboratory 10/83
5/ On Leave from Lawrence Livermore National Laboratory
6/ On Leave from Oak Ridge National Laboratory

INTRODUCTION

The purpose of this report is to provide a convenient compilation and index of the DOE Materials Sciences Division programs. This compilation is intended for use by administrators, managers, and scientists to help coordinate research and as an aid in selecting new programs.

The report is divided into six sections. Section A contains all Laboratory projects, Section B has all contract research projects, Section C has projects funded under the Small Business Innovation Research Program, Section D has information on DOE collaborative research centers, Section E shows distribution of funding, and Section F has various indexes.

Each project in Sections A, B, and C carries a number (at the left hand margin) for reference purposes, e.g., in Section F. The FY 1983 funding level, title, personnel, budget activity number (e.g., 01-2), and key words and phrases accompany the project number. The first two digits of the budget number refer to either Metallurgy and Ceramics (01), Solid State Physics (02), or Materials Chemistry (03). The budget numbers carry the following titles:

01-1 - Structure of Materials
01-2 - Mechanical Properties
01-3 - Physical Properties
01-4 - Radiation Effects
01-5 - Engineering Materials

02-1 - Neutron Scattering
02-2 - Experimental Research
02-3 - Theoretical Research
02-4 - Particle-Solid Interactions
02-5 - Engineering Physics

03-1 - Chemical Structure
03-2 - Engineering Chemistry
03-3 - High Temperature and Surface Chemistry

Section D contains information on special DOE centers that are operated for collaborative research with outside participation.

Section E summarizes the total funding level in a number of selected categories. All projects have been classified under more than one category since the categories are not mutually exclusive.

In Section F the references are to the project numbers appearing in Sections A, B, and C and are grouped by (1) investigators, (2) materials, (3) techniques, (4) phenomena, and (5) environment.

It is impossible to include in this report all the technical data available for such a large program. By the time it could be compiled it would be outdated. The best method for obtaining more detailed information about a given research project is to contact directly the investigators listed.

Preparation of this FY 1983 summary report was coordinated by S. M. Wolf.

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SECTION A

Laboratories

The information on pages 1 through 74 was provided by the Laboratories. Most projects are of a continuing nature although specific projects were concluded and others initiated in FY 1983.

AMES LABORATORY
Iowa State University
Ames, Iowa 50011
R. S. Hansen - Phone (FTS) 865-2770 or 515-294-2770

Metallurgy and Ceramics - 01-
F. V. Nolfi - Phone (FTS) 865-4446 or 515-295-4446

1. SURFACES AND SOLIDIFICATION
R. K. Trivedi, J. T. Mason, A. Roy
Phone: (515)-294-5869
$180,000 01-1

Theoretical and experimental studies of the effect of temperature gradient, growth rate and composition on the stability and steady-state shape of solid-liquid interfaces obtained during controlled solidification. Study of morphological transition from dendritic to cellular to eutectic structure. Experimental work on primary dendrite spacing, eutectic spacing and interface structures in Pb-Sn, Pb-Au, Pb-Pd and Pb-Bi systems. Study of interface stability and morphological characteristics in model transparent material such as succinonitrile and acetone mixture. Microstructure development during amorphous to crystalline transition.

2. MICROSTRUCTURAL CONTROL IN METALS
J. D. Verhoeven, E. D. Gibson
Phone: (515)-294-9471
$285,000 01-1

Production of Nb_3Sn-Cu and V_3Ga-Cu superconducting wire by the in situ process: development of a roll bonding technique to evaluate flux pinning mechanisms and problems in the addition of Sn by the external diffusion method, evaluation of Nb_3Sn filament cross linking within the microstructure, and determination of the effect of residual Si levels on V_3Ga-Cu wire produced by both the in situ and conventional bronze routes. A study of directionally transformed pearlite versus applied stress level and temperature gradient. The mechanical properties of in situ prepared Cu-Ta alloys. Directional solidification studies on segregation in grey and nodular cast iron. Evaluation of microstructural changes in the austempering of nodular cast irons.

3. MATERIALS SCIENCE OF INTERFACES
A. J. Bevolo, F. C. Laabs, L. M. Seaverson
Phone: (515)-294-5414
$ 70,000 01-1

Studies of interfaces using Auger, ELS, and SIMS surface analytical techniques in combination with ion etching. Core level and plasmon spectra of pure and oxidized rare earth metals using ELS and Auger. Effects of tin doping of brass on its corrosion behavior in aqueous salt solutions. Scanning Auger microprobe analysis (350A) of grain boundary inclusions in carbonized low alloy steels and effects of radiation on the competition between C and P grain boundary segregation in iron. Oxidation of liquid and solid tin by ELS. Local chemical state information from Auger lineshape analysis in Fe-B-Be metallic glasses and Mg_2X (X=Si, Ge, Sn, Pb).

AMES LABORATORY (continued)

4. NONEQUILIBRIUM MATERIALS
   J. D. Verhoeven, R. K. Trivedi, A. J. Drehman, A. R. Pelton
   Phone: (515)-294-9471
   $ 70,000 01-1

This is a new area of research which will focus on metallic glasses, metastable crystalline phases and extremely fine microstructural alloys. For initial experiments a high vacuum melt spinning apparatus is being constructed and a directional solidification apparatus modified to achieve very high solidification rates. High speed planar solidification of eutectic Pb-Cd is being studied as well as the microstructure of rapidly crystallized Si-Ge alloys. Future work will include the investigation of a wide range of metallic alloys.

5. MECHANICAL METALLURGY AND MATERIALS RELIABILITY
   O. Buck, J. Kameda, J. Kasichainula, C. V. Owen, D. K. Rehbein,
   B. J. Skillings
   Phone: (515)-294-3930
   $540,000 01-2

Effects of hydrogen on crack initiation in refractory alloys under uniaxial and cyclic loading conditions. Internal friction due to hydrogen in solid solution (in collaboration with the Max-Plank Institute, Stuttgart/Germany) and due to hydrides. Hydrogen induced brittle cracking in low hydrogen solubility bcc metals and alloys. Studies on the effects of radiation-induced defects and solute segregation on intergranular embrittlement. Modeling of hydrogen embrittlement. Microscopic characterization and modeling of the synergetics of stress and deformation on crack initiation under stress corrosion conditions. Ultrasonic characterization of fatigue cracks in alloys exposed to harsh environments. Development of new nondestructive evaluation techniques to determine materials degradation.

6. RARE EARTHS IN STEELS
   M. S. Wechsler
   Phone: (515)-294-5082
   $ 40,000 01-2

Elevated temperature mechanical properties (uniaxial tensile and indentation hardness tests) on ferritic and austenitic steels as a function of rare earth element additions, particularly Y, Ce, and La in concentrations below one percent. Also, irradiation swelling behavior, electron microscopy, and metallography. Application to LMFBR cladding and fusion reactor first wall.

7. SHAPE MEMORY PHENOMENA
   M. S. Wechsler
   Phone: (515)-294-5082
   $ 65,000 01-2

Tensile properties, internal friction, strain and volume change measurements, and resistivity measurements in Ni-Ti as a function of prior transformation fatigue cycling and applied stress.

AMES LABORATORY (continued)

8. THERMODYNAMICS AND PHASE EQUILIBRIA
J. F. Smith
Phone: (515)-294-5083
$ 50,000 01-3

Development of thermodynamic functions for alloy formation in Y-Fe, Y-Co, and Y-Ni systems from electromotive force measurements to test the conflicting predictions of the Bennett-Watson theory and the Miedema theory. Computer analysis of thermodynamic data for the prediction of stable and metastable phase equilibria, glass formation, and control of microstructures.

9. ULTRASONIC MEASUREMENTS
J. F. Smith, R. B. Thompson
Phone: (515)-294-5083 - (515)-294-8252
$ 65,000 01-3

Martensitic transformations in ZrO_2 and HfO_2 are responsible for the sensitivity of these materials to thermal shock. Ultrasonic wave velocities are being measured in yttria stabilized single crystals of ZrO_2 at elevated temperatures to determine the role of the elastic constants in the transformations. Acoustoelastic techniques to determine residual stresses in materials with preferred grain orientations with emphasis on the influence of grain and dislocation structures.

10. TRANSPORT STUDIES
O. N. Carlson
Phone: (515)-294-2375
$200,000 01-3

Study of diffusion and electrotransport of fast diffusing solutes in scandium. Measurement of transport parameters for iron, cobalt and nickel as a function of temperature and determination of activation energy for diffusion. Fast diffusion of cobalt in thorium. Characterization of responsible defect by internal friction studies. Thermotransport of interstitial solutes in one-phase alloys of V and Nb. Mass transport of carbon in two-phase Nb-C and V-C alloys in presence of temperature gradient. Investigation of effect of alloying or impurity elements on ductility transition temperature of Fe-9Cr-1Mo steel using slow, notch-bend and Charpy impact tests. Effect of 500°C aging on ductility of tempered alloys for high purity base alloys and Oak Ridge modified ferritic steel.

11. HYDROGEN IN METALS
D. T. Peterson
Phone: (515)-294-6585
$250,000 01-3

Diffusion, thermotransport, and solubility of H and D in V alloys with Ti, Cr, Nb or O. Photoelectron spectroscopy, and metallography of metal hydrides and solid solutions of H in vanadium base alloys.

AMES LABORATORY (continued)

12. TRANSFORMATION STUDIES AND ORDERED ALLOYS
F. X. Kayser
Phone: (515)-294-5874
$ 80,000 01-3

Resistivity measurements of Fe-Si alloys containing 12 to 26 at.% silicon, from 4.2 to 300 K. Fine-scale structural changes, low temperature phase diagram.

13. RARE EARTH MATERIALS
K. A. Gschneidner, Jr., S. K. Dhar
Phone: (515)-294-2272
$185,000 01-3

The influence of composition and impurities on the quenching of spin fluctuations and other magnetic phenomena in: (1) highly enhanced paramagnets RCo_2 (R=Sc, Y and Lu), Sc and Pd-Ni alloys; (2) valence fluctuation materials $CeSn_x$ ($x = 3$) and $CeSi_x$ ($x = 1.8$) alloys; and (3) itinerant ferromagnets Sc_3In and $ZrZn_2$. Low temperature (1-20 K) - high magnetic field (1-10 T) heat capacity, magnetic susceptibility (1-300 K, 0.9 to 1.5 T), resistance ratio ($\rho_{300}/\rho_{4.2}$), metallography and lattice parameters measurements are being used to characterize the various behaviors. Influence of electron concentration and size on the lattice instability and superconducting properties of rare earth based superconductors: $La_{3-x}S_4$, $La_{3-x}Se_4$ and $(La_{1-x}Th_x)_{3-y}S_4$.

14. NDE MEASUREMENT TECHNIQUES
R. B. Thompson
Phone: (515)-294-8252
$155,000 01-5

Techniques to measure failure related material properties are investigated. Dual objectives of improving understanding of failure mechanisms and inspection reliability. Ultrasonic scattering and harmonic generation studies of fatigue cracks to provide detailed information about closure condition near crack tip and to determine the influence of this condition on detectability.

15. PROPERTIES AND PROCESSING OF CERAMICS
M. F. Berard, M. Akinc, G. W. Jordan, M. D. Rasmussen
Phone: (515)-294-6964
$290,000 01-5

Phase equilibria and electrical conductivity studies in binary and ternary oxides based on HfO_2 and ZrO_2. Effect of processing variables on characteristics of ceramic powders. Influence of hydroxide precursor dewatering treatments on morphology, surface characteristics, compaction and sintering behavior of oxide powders produced from them.

AMES LABORATORY (continued)

16. MATERIALS PREPARATION AND PROCESSING (also see page 180)
F. A. Schmidt, O. D. McMasters
Phone: (515)-294-5236 - (515)-294-3630
$275,000 01-5

Processing of refractory and strategic metals. New process for preparing kilogram quantities of high purity vanadium. New techniques for processing thorium from ThF_4 and for the metallurgical upgrading of cobalt metal. Development of arc melting procedures for preparing Cu-Nb, Cu-Ta and Cu-Mo alloys containing uniform dispersion of the refractory metal. Effect of silicon on the critical current density J_c in V_3Ga. Measurement of diffusion and electrotransport behavior of solutes in rare-earth and refractory metals and the application of these parameters for maximum purification of the host metals. Single crystals (1-2 cm^3) of pure metals, solid solution alloys, intermetallic compounds, both congruent melting and peritectic in nature. Directionally solidified materials for specific applications. Methods available-levitation zone melting in cold crucible, free standing vertical zone melting, Bridgman, Czochralski and strain-anneal recrystallization. Above research being conducted in the Materials Preparation Center described in the Section-Collaborative Research Centers.

Solid State Physics Division - 02-
D. K. Finnemore - Phone (FTS) 865-3455 or 515-294-3455

17. NEUTRON SCATTERING
W. A. Kamitakahara, J. Mizuki, C. Stassis, J. Zarestky
Phone: (515)-294-4224
$350,000 02-1

Study of the lattice dynamics, thermodynamic properties and structural transformations of metals at high temperatures (Mo, fcc La); structure and diffusion in metal hydrides (ScH_x, LaH_x); dynamics and phase transitions of alkali-graphite intercalation compounds; electronic structure and phonon spectra of mixed valence compounds ($CePd_3$, α-Ce, $YbAl_2$); relation of electron-phonon interaction to superconductivity (La,$LaSn_3$). High pressure studies (α-Ce, La).

18. SEMICONDUCTOR PHYSICS
H. R. Shanks
Phone: (515)-294-6816
$220,000 02-2

Preparation and characterization of thin films, rf sputter desposition of amorphous semiconductors including a-Si, a-SiC, a-Ge, a-GeC and AlN, electron beam deposition of Si, heteroepitaxy on compound substrates, surface and interface characterization with LEED, Auger, LEELS, photodeflection and ir absorption spectroscopy for bonding studies, measurements of gap state densities using DLTS and C-V on Schottky barriers.

AMES LABORATORY (continued)

19. SUPERCONDUCTIVITY

D. K. Finnemore, J. R. Ostenson, E. L. Wolf, T. P. Chen, Y. Q. Zhou
Phone: (515)-294-3455
$390,000 02-2

Electron tunneling spectroscopy and surface physics studies of strong coupled transition metal superconductors, including alloys and compounds. Conventional and proximity electron tunneling spectroscopy (PETS) of the electron-phonon spectrum $\alpha^2F(\omega)$. Auger electron spectroscopy (AES), electron energy loss spectroscopy (ELS) and ultraviolet photoemission spectroscopy (UPS). Fundamental studies of superconductivity in inhomogeneous materials; supercurrents in normal metals near a superconductor normal metal boundary; quantum interference phenomena and studies of the motion quantized vortices in SNS junctions; development of superconducting composites suitable for large scale magnets in the 8 to 16 Tesla range; practical studies to improve wire fabrication techniques; development of magnetic shielding devices.

20. OPTICAL AND SPECTROSCOPIC PROPERTIES OF SOLIDS AND LIQUIDS

D. W. Lynch, C. G. Olson, D. M. Wieliczka
Phone: (515)-294-3476
$350,000 02-2

Electron photoemission and optical properties (transmission, reflection, EXAFS, thermoreflection, thermotransmission, of solids in the near infrared, visible, vacuum ultraviolet and soft X-ray region using synchrotron radiation): transition metal alloys and compounds (e.g., NiAl, Fe_3Al), layered transition metal chalcogenides ($MoSe_2$), Ce; electroreflectance of Ag in electrolytes. Raman Scattering.

21. NEW MATERIALS AND PHASES

R. N. Shelton, C. A. Swenson, R. G. Barnes, M. S. Anderson, P. Klavins, D. R. Torgeson, J. S. Schilling
Phone: (515)-294-5435
$440,000 02-2

Synthesis and characterization of new ternary compounds such as Chevrel phases, ternary transition metal borides and rare earth transition metal silicides and phosphides. Study of the physical properties of these new materials, such as microhardness, phase equilibria and their refractory nature, and high temperature behavior. Properties of new ternary phases at low temperatures, including magnetic susceptibility, transport properties, heat capacity, crystallographic phase transformations, coexistence of superconductivity and long range magnetic order. High pressure equations of state of new materials, elementary solids (alkali and alkaline earth metals); effects of hardness on thermal expansivities of technical materials (beryllium copper); low temperature expansivity of materials (Lu) containing hydrogen. Applications of NMR to hydrogen embrittlement of refractory metals (V, Nb, Ta) and alloys (V-Ti, Nb-V), trapping of hydrogen of interstitial impurities in these metals, structural and electronic characterization of hydrogenated amorphous silicon films.

AMES LABORATORY (continued)

22. MATERIALS FOR HYDROGEN STORAGE

R. G. Barnes, J. D. Corbett, K. A. Gschneidner, Jr., W. A. Kamitakahara,
D. T. Peterson, R. J. Schoenberger
Phone: (515)-294-4754

$180,000 02-2

Interdisciplinary study of metal-hydrogen interactions for development of better hydrogen-storing materials. Materials studied include hydrides of transition metals (e.g., YH_2), refractory alloys (e.g., V-Ti-H), rare-earth-transition metal compounds (e.g., $Y(Al,Ni)_5$-H), and low-valent and lower-dimensional compounds of Group III and IV metals (e.g., LaCl-H, ZrCl-H). Properties and methods include hydrogen locations, super structures, phase transformation, electronic density-of-states, hydriding kinetics, enthalpies of hydride formation, hydrogen diffusion, low-temperature heat capacity, X-ray and neutron diffraction, nuclear magnetic resonance, XPS and UPS.

23. X-RAY DIFFRACTION PHYSICS

J.-L. Staudenmann
Phone: (515)-294-3585

$200,000 02-2

X-ray diffraction studies of martensitic phase transitions (V_3Si and Fe-C) and electron charge densities; small angle scattering, EXAFS, microdiffraction. Studies of electron density near interstitial impurities. MATRIX PRT beam line at NSLS.

24. ELECTRONIC AND MAGNETIC PROPERTIES

B. N. Harmon, K.-M. Ho, M. Luban, D. Misemer, M. Nolan
Phone: (515)-2984-7712

$400,000 02-3

Theory of phonon anomalies, lattice instabilities and soft modes in metals and their relation to the electron-phonon interaction and superconductivity (Nb, Mo, Zr, Ti). Total energy frozen phonon calculations for high temperature bcc to ω-phase transition and lattice dynamics. Surface electronic structure of metal electrodes (e.g., Ag), electroreflectance, and microscopic properties of the metal-electrolyte interface. Static and dynamic properties of mixed valence compounds ($CeSn_3$). Electronic properties and chemical bonding of transition and rare earth metal compounds (ZrB_2, $ZrSe_3$, ZrS, TiS, PtTe, LaH_2, LaH_3, ScH_2). Vacancy formation and ordering (Sc_xS). Renormalization group studies of phase transitions. Electron localization in disordered metals.

25. OPTICAL AND SURFACE PHYSICS THEORY

R. Fuchs, K. M. Ho, S. Auluck
Phone: (515)-294-3675

$150,000 02-3

Optical properties of metals, semiconductors, and insulators; studies of surfaces, thin films, layered systems, small particles, and powders. Differential surface reflectance spectroscopy. Raman scattering from molecules adsorbed on metal surfaces. Photoemission and electroreflectance with emphasis on surface states. Photoemission into liquid electrolytes and related catalytic, electrochemical, adsorption, and corrosion effects; anodic photocurrents; the liquid-metal interface.

AMES LABORATORY (continued)

26. SUPERCONDUCTIVITY THEORY
J. R. Clem, V. G. Kogan
Phone: (515)-294-4223
$110,000 02-3

Electrodynamics of superconductor-normal metal composites; properties of current-carrying type-I and type-II superconductors containing magnetic flux; induced voltages and energy dissipation due to flux motion; flux-flow voltage noise; vortex nucleation and surface pinning; flux-line cutting in arrays of nonparallel vortices; critical currents and flux pinning in inhomogeneous superconductors; instabilities; ac losses; superconducting magnetic shielding.

Materials Chemistry Division - 03-
L. E. Burkhart - Phone (FTS) 865-8074 or 515-294-8074

27. X-RAY AND NEUTRON CRYSTALLOGRAPHY
R. A. Jacobson, B. J. Helland
Phone: (515)-294-8444
$185,000 03-1

Development of diffraction techniques for single crystal and non-single crystal specimens; indirect methods and refinement techniques; operation of X-ray characterization facility; radial distribution function analysis of amorphous scattering from coal; structural studies of intramolecular solid state interactions which modify properties of parent species; metal complex structures with emphasis on model homogeneous catalysts and polymetal species; coordination numbers and oxidation states for complex molybdates and sulfides using EXAFS.

28. METAL-METAL BONDING IN NEW SOLID STATE MATERIALS
J. D. Corbett
Phone: (515)-294-3086
$170,000 03-1

Materials preparation and characterization of new types of reduced inorganic compounds stable at high temperature (e.g., of Sc, Y, Ti, Zr, Nb, rare earth elements); extended metal-metal bonding; hydrogen storage potential of new types of reduced compounds; chemistry of stress-corrosion-cracking by zirconium; homopolyatomic ions; charge transfer and bonding in Zintl-type phases; crystal structures; photoelectron spectroscopy; electronic structure.

29. STRUCTURE-PROPERTY RELATIONS IN HEAVY TRANSITION METAL PHASES
R. E. McCarley
Phone: (515)-294-8680
$165,000 03-1

Chemistry of heavy transition elements, especially Nb, Ta, Mo, and W. Compounds with strong metal-metal bonding in discrete cluster units and phases with extended metal-metal bonded chains. Ternary and quaternary oxides of molybdenum with metal-clusters and chains. Chemistry of new sulfide compounds with relation to hydrodesulfurization catalysis. Studies of structure and bonding in new oxide and sulfide compounds, and their relationship to physical properties such as electrical and ionic conductivity, mechanical strength, and catalytic activity.

AMES LABORATORY (continued)

30. RECOVERY OF METALS FROM FLY ASH AND OTHER WASTE MATERIALS
G. Burnet, M. J. Murtha
Phone: (515)-294-5840
$170,000 03-2

Recovery from power plant fly ash of iron oxide by magnetic separation and of alumina using calcination; use of magnetic fraction for heavy media in coal preparation plants and source of iron ore; utilization of wastes from fly ash processing plants; X-ray studies of complex metal phosphates found in Portland cement-type wastes from fly ash processing plants; recovery of metals from other fuel processing wastes.

31. PARTICULATE PROCESSING
L. E. Burkhart, A. Cahill
Phone: (515)-294-8074
$290,000 03-2

Methods for the preparation of ceramic powders; reaction kinetics and control of nucleation, growth rate, and particle size distribution in both liquid phase and vapor phase operations for preparing particulate materials; quantitative description of particle morphology; techniques for modifying particle morphology; quantitative measurement of strength of particle agglomerates; X-ray studies of particulate materials.

32. HIGH TEMPERATURE CHEMISTRY OF REFRACTORY MATERIALS
H. F. Franzen, Bernd Harbrecht
Phone: (515)-294-5773
$245,000 03-3

Fracture and bonding in refractory and corrosion-resistant compounds, particularly metal-rich transition metal chalcogenides (Sc-S and Ta-S), phosphides and aluminides (Zr-Al); stability, phase equilibria, order-disorder transitions, X-ray diffraction, photoelectron spectroscopy, and mass spectrometry studies at high temperatures; band structure and electronic properties of transition-metal sulfides.

33. SURFACE CHEMISTRY AND CATALYSIS
R. S. Hansen, K. G. Baikerikar, D. C. Johnson
Phone: (515)-294-2770
$315,000 03-3

Heterogeneous catalysis, reactions at clean surfaces (including alloy surfaces) associated with coal liquefaction and gasification (e.g., methanation reaction on ruthenium and hydrodesulfurization using non-stoichiometric rare earth sulfides); field emission, flash desorption, LEED and Auger spectroscopy techniques for studying reaction kinetics and composition of surface phases resulting from the interaction of gases such as CO and H_2 on catalyst single crystal faces; electrical double layer properties and their alteration by adsorption, electrochemistry associated with stress corrosion cracking, electrocatalysis at binary electrode surfaces for control of toxic or mutagenic organic molecules (nitrosoamines, polynuclear compounds) in wastes; preparation and electrochemistry of layered chalcogenide photochemical converters (e.g., MoS_2, $MoSe_2$, WSe_2).

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

Materials Science & Technology Division - 01 -

B. R. T. Frost - Phone (FTS) 972-4928 or 312-972-4928
F. Y. Fradin - Phone (FTS) 972-4925 or 312-972-4925
H. Wiedersich - Phone (FTS) 972-5079 or 312-972-5079
F. A. Cafasso - Phone (FTS) 972-4542 or 312-972-4542

34. **LAYERED AND THIN FILM MATERIALS**
M.B. Brodsky, S.D. Bader, M.H. Grimsditch, R.C. Haushalter,
I.K. Schuller, C.S.L. Chun, H.C. Hamaker, G.W. Zajac, G.-G. Zhen
Phone: (312)-972-5016
$ 981,000 01-1

Studies of novel materials properties obtained by thin film techniques—epitaxial sandwiches, multilayered coherent samples and metallic overlayers; room temperature preparation of metallic materials, often metastable and glassy, via Zintl ions. Preparation techniques include atomic (molecular) beam epitaxy and sputter deposition. Materials characterization methods involve magnetic and superconducting properties at low temperatures; atomic structure by TEM and X-ray and electron diffraction; electronic structure changes via AES, UPS, XPS, chemical bonding and theoretical calculations; and vibrational and magnetic excitations by Raman and Brillouin light scattering, neutron scattering and ELS; interface phenomena.

35. **DEFECTS IN METALS**
R.W. Siegel, R. Benedek, M.J. Fluss, N.Q. Lam, J.N. Mundy,
J.E. Robinson, L.C. Smedskjaer, D.G. Westlake, B. Chakraborty,
G.D. Loper
Phone: (312)-972-4963
$1,223,000 (Does not include H in metals effort) 01-3

Research on the nature and physical properties of intrinsic and extrinsic atomic defects and their interactions in metals, and the relationship between these and the atomic mechanisms of diffusion under equilibrium and non-equilibrium conditions and the properties of metallic materials; investigations of atomic and defect diffusivities; equilibrium defect formation and concentrations; interactions of atomic defects with one another, with solute atoms, and with interfaces and surfaces; and hydrogen interactions with metallic systems; studies of metals (including refractory bcc metals), alloys, intermetallic compounds, and amorphous metallic systems with experimental techniques such as positron annihilation spectroscopy, radiotracer diffusion, resistometry, transmission and scanning electron microscopy, neutron and x-ray diffraction, and ion-scattering spectroscopy, and the complementary theoretical methods of molecular statics and dynamics, computer modeling, and electronic structure calculations.

ARGONNE NATIONAL LABORATORY (continued)

36. DEFECTS IN CERAMICS
N.L. Peterson, K. Hoshino, K.L. Merkle, G.E. Murch, J.L. Routbort,
J. Sasaki, M. P. Thomas, D. Wolf
Phone: (312)-972-4955
$825,000 01-3

Diffusion mechanisms and point-defect studies in metal oxides as a function of oxygen-partial pressure at high temperatures using tracer diffusion, conductivity and TEM techniques; impurity-diffusion mechanisms, defect-solute interactions and defect clustering in oxides; computer modeling of diffusion processes at dislocations and in nonstoichiometric compounds; TEM studies of dislocation structures in grain boundaries in oxides; theory of defect kinetics, vibration entropy, and atomic structure in grain boundaries; grain-boundary diffusion in metal oxides; diffusion mechanisms and impurity interactions in mixed-alkali silicate, alkali-borate, alkali-germanate, and alkali-silicon-sulfur glasses; effect of nonstoichiometry and defect clusters on mechanical deformation of oxides; preparation of single and bicrystals of metal oxides.

37. NEUTRON IRRADIATION STUDIES
M.A. Kirk, R.C. Birtcher, S. Egusa, and B.A. Loomis
Phone: (312)-972-4998
$526,000 01-4

Fast neutron irradiation effects in solids studied using the Radiation Effects Facility at IPNS and in-situ ion irradiation in the HVEM facility; the structure and properties of cascades, interactions of free interstitials and vacancies and their clusters in metals and alloys using resistivity, ordered alloys, TEM, and electron irradiation probe techniques; interactions of gliding dislocations with neutron irradiation produced defect structures studied in the HVEM in niobium, vanadium and their alloys; the collapse of defect cascades to dislocation loops studied in the HVEM in Cu_3Au and Fe following low temperature in-situ ion irradiations; low temperature defect production and annealing in semiconductors studied with resistivity and deep level transient spectroscopy; superconducting property changes in various metallurgical states of Nb-Ti following fast neutron irradiation at 5K; changes in mechanical properties of organic composite insulators following fast neutron irradiations at 5 and 300K.

ARGONNE NATIONAL LABORATORY (continued)

38. KINETICS AND ION IRRADIATION
L.E. Rehn, C.W. Allen, R.S. Averback, J. Don, R.C. Frank, U.F. Kocks, S. Majumdar, P.R. Okamoto, R.B. Schwarz, N.J. Zaluzec
Phone: (312)-972-5021
$1,023,000 01-4

Investigations of mechanisms leading to the formation of defect aggregates, precipitates and other inhomogeneous distributions of atoms in solids with and without displacement-producing irradiation; surface layer modification of alloys by ion implantation, ion-beam mixing, and sputtering; solute segregation to internal and external defect sinks; effects of irradiation on alloy composition and microstructure; in-situ studies of ion and electron bombardment in the High Voltage Electron Microscope; analytical electron microscopy; mechanistic studies of deformation and mechanical strengthening in alloys; theoretical and experimental investigations of solute hardening and dynamic strain aging; radiation sources include HVEM-2MV Tandem facility and two 300 kV ion accelerators.

39. HIGH VOLTAGE ELECTRON MICROSCOPE TANDEM FACILITY (also see page 170)
A. Taylor
Phone: (312)-972-5109
$625,000 01-4

Operation and development of 1.2 MeV High Voltage Electron Microscope Facility with in-situ capability for ion implantation, ion damage, and ion beam analysis; the HVEM is currently being utilized for research programs in mechanical properties, radiation damage, oxidation and hydrogenation effects; specimen stages for heating (1000°C), cooling (9°K), straining, gaseous environments and for the ion-beam interface with a 300 kV ion accelerator and a 2 MV tandem accelerator are available for in-situ implantations and irradiations; approximately 50% of the HVEM usage is by non-ANL scientists on research proposals approved by a steering committee for the HVEM that meets every six months.

ARGONNE NATIONAL LABORATORY (continued)

40. OXIDATION STUDIES
N.L. Peterson. D.J. Baxter, K. Hoshino, W.E. King, K. Natesan, S.J. Rothman, J. Sasaki
Phone: (312)-972-4955
$623,000 01-5

Point defects and diffusion mechanisms in protection-oxide scales; grain-boundary diffusion in pure- and doped-protective-oxide materials; studies of adhesion and morphology of oxide scales on crystalline and amorphous alloys using analytical-electron-microscopy techniques; mechanisms and kinetics of oxide film breakdown in bioxidant atmospheres.

41. NEUTRON AND X-RAY SCATTERING
D.L. Price, T.O. Brun, J.E. Epperson, J. Faber, Jr., G.P. Felcher, J.D. Jorgensen, P.R. Roach, S.K. Sinha, M.H. Mueller, M. Loewenhaupt, B.K. Sarma, C.K. Saw
Phone: (312)-972-5475
$1,397,000 02-1

Use of neutron and x-ray scattering techniques in the study of the properties of condensed matter; instrument development and interactions with university and industrial users at IPNS-I and NSLS; hydrogen in metals, magnetism of intermetallic compounds, alloy decomposition, silicate and chalcogenide glasses, residual stresses in deformed materials, surface magnetism, ternary superconductors, atomic momentum distributions in quantum systems, and nuclear magnetism at ultralow temperatures.

42. CHEMICAL AND ELECTRONIC STRUCTURE
J.M. Williams, C.D. Carlson, R.J. Thorn, A.J. Schultz, M. Beno, P. Leung, H. Horiuchi
Phone: (312)-972-3464
$853,000 02-1

Synthesis and characterization of new materials, especially synthetic organic metals possessing novel electrical properties, dielectric materials, fast oxygen-ion conductors, and compounds that behave as catalysts or model catalysts. Continuing development of the neutron time-of-flight single-crystal diffractometer (SCD), and the U.S. university-industrial users group at the Intense Pulsed Neutron Source. Structure-property relationships for synthetic metals based on TMTSF (tetramethyltetraselenafulvalene) and for organometallic complexes and hydrides which may be active or model catalysts. Variable temperature diffuse scattering and crystal structure studies at the SCD. Development of a very low-temperature (10K) single crystal X-ray facility for electron density and structural studies which require neutron and X-ray data collected at identical temperatures.

ARGONNE NATIONAL LABORATORY (continued)

43. SUPERCONDUCTIVITY AND MAGNETISM
B.D. Dunlap, F. Behroozi, G.W. Crabtree, A.J. Fedro, F.Y. Fradin, K.E. Gray, D.G. Hinks, W.P. Joss, H.C. Li, G.K. Shenoy, A. M. Umarji
Phone: (312)-972-5538
$962,000 02-2

Experimental and theoretical investigations of the magnetic and superconducting properties of materials. Experimental techniques utilized include de Haas-van Alphen effects, Mössbauer spectroscopy, nuclear magnetic resonance, transport measurements, magnetization and susceptibility, electron tunneling, EXAFS and XANES, materials preparation and characterization, and collaborative efforts using neutron scattering. Current topics of interest include: investigations of the relationships between superconductivity and magnetism in the RRh_4B_4 system (R = rare-earth); the role of oxygen impurities in establishing superconducting properties of Chevrel phase systems; superconductivity and magnetism in Heusler phase alloys; Fermi surface studies of narrow band systems, including mixed valence and Kondo lattice phenomena; theoretical investigation of the effect of superconductivity on magnetic exchange coupling; investigation of the electronic properties of organic superconductors; structural studies of chalcogenide gases; design and construction of a soft x-ray beam line at NSLS.

44. MATERIALS PREPARATION AND CHARACTERIZATION AND FAST ION TRANSPORT IN SOLIDS
S. Susman, T. O. Brun, C.J. Delbecq, J.A. McMillan, T. Tokuhiro
Phone: (312)-972-5470
$419,000 02-2

Preparation of metal, insulator and semiconductor single crystals with documented physical and chemical properties; solidification of vitreous systems with characterized and reproducible compositions and thermal histories. Investigations of mechanisms involved in purification, crystal growth, phase transformations and solidification. Materials of current interest include semiconducting chalcogenide glasses, Zintl-phase compounds, complex phosphates and oxides and cyanides. Basic studies are conducted in the microscopics of charge and mass transport in solid electrode and electrolyte materials utilizing neutron diffraction, nuclear magnetic resonance, ionic conductivity, EXAFS and optical spectroscopy. Fast ion transport is examined in mixed electronic and ionic conductors, in skeleton framework compounds and in fast-ion glasses. These include ternary sulphide glasses, Li-Al alloys, NASICON analogs, NASIGLAS, and both crystalline and vitreous β-eucryptites.

ARGONNE NATIONAL LABORATORY (continued)

45. ELECTRONIC STRUCTURE AND BONDING
D.J. Lam, A. T. Aldred, A. J. Arko, S.-K. Chan, G.S. Knapp, J. McMillan, M.V. Nevitt, B.W. Veal, Q.Q. Zheng
Phone: (312)-972-4966
$1,309,000 02-2

Experimental and theoretical studies of electronic structure and its relationship to physical and chemical properties and bonding in solids; x-ray photoemission (XPS) and x-ray absorption (XANES and EXAFS) spectroscopic studies of structural and electronic properties of actinide oxides in silicate glasses; application of differential thermal analysis and Raman spectroscopy to study the devitrification of silicate glasses containing actinides; crystal chemistry and structural stability of complex metal oxides; XPS and XANES studies of structural and electronic properties of ABO_4 compounds; thermal and lattice properties study of ABO_4 compounds using heat capacity, EXAFS, Raman scattering and inelastic neutron scattering measurements; theoretical studies of electron spectra and bonding of ABO_4 and AB_2O_4 compounds; development of molecular cluster code to calculate total energy of embedded AB_2O_4 clusters; formulation of the theory of EXAFS and XANES for heavy elements; angle resolved photoemission spectroscopy and de Haas-van Alphen studies of the electronic band structure of actinide intermetallic compounds; magnetization and photoemission spectroscopy (UPS and XPS) studies of actinide intermetallic compounds to determine the electronic configuration and stability of 5f electron states.

46. THEORETICAL RESEARCH - CONDENSED MATTER THEORY
D.Y. Smith, L. Guttman, R. Kalia, D. Koelling, A. Rahman, P. Vashishta
Phone: (312)-972-5481
$731,000 02-3

A broad activity in condensed matter theory focusing on statistical physics, electronic structure, and the defect solid state. Current areas of study include: molecular dynamics calculations to model structural phase transitions, melting and nucleation, and fast ion transport in solids; electronic structure calculations of narrow-band materials, including actinides and mixed valence systems; many-body effects in semiconductors, especially Green's function Monte Carlo simulation of multi-exciton complexes and the electron-hole liquid, optical and x-ray properties of materials, the electronic structure of defects in insulators and electron solvation in molten salts; calculations of the spatial and electronic structure of amorphous semiconductors and covalent glasses.

ARGONNE NATIONAL LABORATORY (continued)

47. GEOPHYSICAL PROSPECTING WITH SQUIDS
R.T. Kampwirth, I.K. Schuller
Phone: (312)-972-5521
$178,000 02-5

The goal of this program is to develop and evaluate instrumentation and data analysis techniques for the location of subsurface hydrocarbon deposits using Superconducting quantum interference Devices (SQUIDS) in conjunction with remote reference Controlled Source Sounding techniques. These results will be compared with Magnetotelluric measurements and well log data where available. Preliminary instrumentation evaluation at a known oil-bearing site has been completed. Data reduction and analysis is in progress.

48. THERMODYNAMICS AND STRATEGIC MATERIALS
M. Blander, L.A. Curtiss, P.A.G. O'Hare, G.K. Johnson, V.A. Maroni, M.-L. Saboungi, J.L. Settle, R.M. Yonco
Phone: (312)-972-4548
$722,000 03-02

Experimental and theoretical studies aimed at investigating important thermodynamic, structural, and solution properties of inorganic materials including strategic and critical materials and minerals. Application of spectroscopic methods to the study of solvation and coordination chemistry of transition metals in low-melting ionic salts and other nonaqueous solvents. Exploration of new complexation methods for the dissolution of strategic and valuable metals from naturally occurring minerals and from effluent materials (e.g., fly ash) by use of spectroscopic, emf, and analytical measurements as well as theoretical models. Thermochemical measurements of the enthalpies of formation, standard entropies, and Gibbs energies of formation of strategically significant compounds that occur in both fuel and nonfuel materials and minerals. Quantum mechanical and statistical mechanical calculation of thermodynamic functions and structures of vapor complexes.

49. CHEMISTRY OF MATERIALS
R. Kumar, B. Holt, Dr. Drapcho, S. Johnson
Phone: (312)-972-4342
$515,000 03-02

Formation mechanisms of atmospheric sulfate and nitrates, and their relationship to acid precipitation chemistry. Stable oxygen isotope ratio measurements; in-situ sampling and real-time analysis and characterization of particulates; infrared spectroscopic and chemiluminescent instruments for atmospheric SO_x and NO_x species analysis; in-situ investigations of gas (SO_2, NO_x) particle reactions using an ATR-IR technique and studies of the effects of surface chemistry on sulfate and nitrate formation and neutralization mechanisms.

ARGONNE NATIONAL LABORATORY (continued)

50. ELECTROCHEMISTRY AND ENERGY SYSTEMS
M. Blander, L.A. Curtiss, G.K. Johnson, V.A. Maroni
C. A. Melendres, Z. Nagy, M.-L. Saboungi, J.L. Settle
Phone: (312)-972-4547
$603,000 03-02

Experimental electrochemical and spectrochemical measurements as well as quantum mechanical calculations to examine the mechanisms and rates of electron transfer reactions involving iron phthalocyanine and other compounds as catalysts in the cathodic reduction of O_2 at electrode surfaces. Electrochemical relaxation techniques for very fast reactions; examination of the kinetics of anodic dissolution, of incipient passivation, and of other elementary steps in corrosion; kinetics and mechanisms of inhibition. Investigation of ordered and associated solutions by a variety of experimental and theoretical techniques including emf, solubility, calorimetry, neutron diffraction, molecular dynamics, and quantum mechanical calculations. Some materials under study include chloroaluminates, ionic alloys (such as Na-Pb and Rb-Au) and metal-salt systems (such as Rb-RbCl). Spectroelectrochemical studies of polysulfide formation in aprotic media.

51. PARTICLE-SURFACE INTERACTION CHEMISTRY AND CATALYSIS
D.M. Gruen, B. Abraham, W.F. Calaway, E. Iton, A. Krauss, K. Miyano,
C. Melendres, M. Mendelsohn, T. I. Morrison, M.J. Pellin, C.E. Young,
G.J. Lamich
Phone: (312)-972-3513
$1,138,000 03-03

Static mode laser fluorescence spectroscopy of sputtered products from clean and adsorbate covered surfaces: a new tool for determining surface structures. Excited state and velocity distributions of sputtered atoms. Surface segregation kinetics in dilute alloy systems during energetic particle bombardment. Electronic structures of matrix isolated ligand-free transition-metal clusters. Generation of new metal-bearing shape selective medium pore zeolite catalysts useful in Fischer-Tropsch syntheses. Characterization of catalysts by EPR, FMR, PAS, and DTA techniques. Synchrotron radiation studies of catalytic materials. In-situ spectroscopic investigation of the anodic corrosion of metals. Investigation of the surface properties of polymeric monolayers on metals by nonlinear optical processes. Viscoelastic properties of monomolecular films spread on aqueous substrates.

ARGONNE NATIONAL LABORATORY (continued)

52. INTENSE PULSED NEUTRON SOURCE PROGRAM (also see page 162)
G.H. Lander, B.S. Brown, J.M. Carpenter, C.W. Potts, A.W. Schulke,
T.G. Worlton, R.K. Crawford, F.J. Rotella, M.H. Mueller
Phone: (312)-972-5518
$4,600,000 02-1

The IPNS Program has the goal of providing an intermediate-flux pulsed spallation neutron source for condensed matter research with neutron scattering and irradiation techniques. The IPNS-I facility is equipped with 7 insruments which are regularly scheduled for users, a low-temperature irradiation facility, and 3 beam tubes which are assigned to special experiments. Routine operation started in November 1981. The facility is run as a national facility in which experiments are selected on the basis of scientific merit by a nationally constituted Program Committee. Aproximately 50 experiments, many involving participants in collaborative research from Universities and indusry were performed in the period Octoer 1981-March 1982, and another 60 will be scheduled for the next 6 months. Relevant Argonne research programs appear under the neutron activities of the Materials Science and Technology Division of Argonne National Laboratory.

BROOKHAVEN NATIONAL LABORATORY
Upton, Long Island, New York 11973

Corrosion Science Group - 01 -

J. R. Weeks - Phone (FTS) 666-2617 or 516-282-2617
A. N. Goland - Phone (FTS) 666-3819 or 516-282-3819

53. INTERGRANULAR STRESS CORROSION
H. S. Isaacs, K. Sieradzki, L. C. Newman.
Phone: (FTS) 666-4516 or 516-282-4516

$370,000 01-2

Mechanistic aspects of intergranular corrosion cracking and hydrogen embrittlement of iron, nickel, and copper base alloys in ambient and high temperature water. Studies of effects of heat treatment, stress, surface treatment, and sulfur compounds in solution. Electrochemical techniques include ac impedance, polarization measurements and _in situ_ surface scanning for determining location of heterogeneities, hydrogen permeation, and dissolution in simulated crack environments. Mechanical tests include acoustic emission, stress cycling, crack growth rate measurements, constant elongation rate testing and effects of surface damage on cracking and repassivation. Surface analysis includes determination of grain boundary segregation and oxide films using scanning transmission microscopy, and x-ray photoelectron spectroscopy.

Materials Science Division - 01 -

A. N. Goland - Phone (FTS) 666-3819 or 516-282-3819
M. Suenaga - Phone (FTS) 666-3518 or 516-282-3518

54. BASIC PROPERTIES OF AMORPHOUS SEMICONDUCTOR MATERIALS
P. E. Vanier, R. R. Corderman, F. J. Kampas.
Phone: (FTS) 666-3535 or 516-282-3535

$260,000 01-1

Investigations of the growth, structure, and properties of plasma-deposited thin-fim amorphous semiconductors. Studies by optical and mass spectroscopy of processes in the plasma and their relation to film growth and defect formation. Studies of film structure and morphology by electron and optical microscopy, positron annihilation, and x-ray absorption fine structure EXAFS. Studies of chemical bonding by infrared absorption and electron spin resonance. Measurement of photoelectronic properties and their correlation with structural and bonding characteristics.

BROOKHAVEN NATIONAL LABORATORY (continued)

55. RELATIONSHIP BETWEEN PROPERTIES AND STRUCTURES
D. O. Welch, M. Suenaga, J. Tafto, N. Higuchi.
Phone: (FTS) 666-3517 or 516-282-3517
$380,000 01-3

Fundamental properties of high critical-temperature and critical field superconductors; effects of strain, disorder, and lattice defects on superconducting properties; theoretical models of interatomic forces, lattice defects, and diffusion kinetics in A15 compounds; annealing and layer-growth kinetics in A15 compounds; studies by electron microscopy of lattice defects in superconducting compounds; flux pinning; properties of composite superconductors; new methods of fabricating superconducting materials.

56. PHYSICAL PROPERTIES
M. S. Pick (on leave), T. H. Metzger, S. M. Heald, D. O. Welch.
Phone: (FTS) 666-3517 or 516-282-3517
$450,000 01-3

Studies of physical and metallurgical factors which influence the behavior of interstitial solutes in metals and alloys; studies of the role of microstructure, lattice defects, alloying effects, and surface properties on the thermodynamics, kinetics, and mechanisms of hydrogen uptake and release in transition metals, solid solutions, and intermetallic compounds; effect of dissolved hydrogen upon fracture strength; structural and microstructural studies of metal-interstitial systems using optical, neutron, and x-ray diffraction, EXAFS, electron microscopic, nuclear depth profiling, and surface sensitive techniques; statistical mechanics of metal-interstitial systems.

57. ELECTROCHEMICAL PROPERTIES OF INTERFACES
W. E. O'Grady.
Phone: (FTS) 666-2829 or 516-282-2829
$100,000 01-3

The role played by the structure, chemical composition, and oxidation states of the surface in electrode reactions is being studied. Electrochemical techniques combined with low energy electron diffraction, Auger electron spectroscopy, x-ray photoelectron spectroscopy, and EXAFS are being used. High surface area catalysts prepared by various techniques including ion implantation are also being investigated in an effort to bridge the gap between studies on well defined single crystals and those on microcatalyst particles.

58. PROPERTIES OF DEFECTS IN MATERIALS
C. L. Snead, Jr.
Phone: (FTS) 666-3502 or 516-282-3502
$290,000 01-4

Effects of different types of irradiation on critical properties of type-II superconductors; electron, reactor neutron, 14-MeV neutron, 17-MeV, 800-MeV and 30-GeV proton irradiations; Nb-Ti, and A15 superconductors; defect and microstructure changes in irradiated materials; enhanced diffusion applied to A15 superconductors solid-state process; application of positron annihilation to defect studies: irradiation-induced defects, and gases in metals. Mechanical properties of various materials using internal friction and dynamical Young's modulus techniques.

LABORATORIES

BROOKHAVEN NATIONAL LABORATORY (continued)

Department of Chemistry -02-

A. P. Wolf: (FTS) 666-4397 or 516-282-4397

59. NEUTRON SCATTERING
L. M. Corliss, J. M. Hastings, R. Thomas
Phone: (FTS)-666-4376 or (516)-282-4376

$400,000 02-1

Neutron scattering is used in this program to study the statistical mechanics of phase transitions, the dynamical properties of solids, properties and spin configurations of magnetic materials, and also crystal structures where relevant to the general program.

The strong interaction of neutrons with vibrational, rotational, and diffusive modes in crystals makes inelastic neutron scattering an excellent probe of atomic motion in solids and particularly well adapted to studies of phonons and hydrogen motion. In the case of magnetic systems one can measure the spatial distribution of magnetization and the behavior of spontaneous fluctuations, both of which are essential to understanding magnetic phase diagrams and their associated first- and second-order transitions. Because of the universal nature of critical phenomena, information gained from magnetic systems can be readily transferred to the study of other systems exhibiting second-order phase transformations, such as simple and multicomponent liquids, alloy systems, and superfluids.

Department of Physics -02-

V. J. Emery: (FTS) 666-3765 or 516-282-3765

60. MAGNETIC AND STRUCTURAL PHASE TRANSITIONS
G. Shirane, S. M. Shapiro, G. Aeppli, J. D. Axe, D. Belanger,
O. Steinsvoll, J. Wicksted
Phone: (FTS) 666-3732 or 516-282-3732

$1,155,000 02-1

Neutron scattering studies of the structure and dynamics of phase transitions. Random magnetic systems, magnetic superconductors, low dimensional charge density waves, incommensurate systems and soft modes in solids.

61. ELEMENTARY EXCITATIONS AND NEW TECHNIQUES
G. Shirane, L. Passell, B. H. Grier, P. Böni, C. F. Majkrzak,
H. Yoshizawa
Phone: (FTS) 666-3732 or 516-282-3732

$1,400,000 02-1

Neutron scattering studies of low-lying excitations in solids and overlayer films, electron-phonon interactions in metals and lattice dynamics of metal hydride systems. Development of efficient neutron polarizer and new devices for beam modulation.

BROOKHAVEN NATIONAL LABORATORY (continued)

62. EXPERIMENTAL RESEARCH - X-RAY SCATTERING

D. E. Moncton, K. D'Amico, B. C. Frazer (on leave), L. D. Gibbs, J. B. Hastings, H. Moudden
Phone: (FTS)-666-2741 or (516)-282-2741

$ 750,000 02-2

Structural and dynamic properties of condensed matter systems, studied by x-ray and neutron scattering; phase transition and new states of matter particularly in two-dimensional (2D) systems 2D melting, commensurate-incommensurate transitions and molecular orientational transitions. Extension to single crystal surfaces under ultra high vacuum conditions is in progress; study of the structure of atomic microclusters produced in nozzle beams; research and development studies of synchrotron instrumentation for NSLS experiments.

63. EXPERIMENTAL RESEARCH - LOW ENERGY - PARTICLE INVESTIGATIONS OF SOLIDS

K. G. Lynn, D. Chen (CCNY); D. Fischer, (SUNY, Stony Brook), W. J. Kossler (College of William and Mary; A. P. Mills, Jr. (Bell Labs); I. K. MacKenzie (U. Guelph, Canada); B. Nielsen, L. Roellig (CCNY); P. J. Schultz, C. L. Snead, Jr. (DAS); A. Vehanen (U. of Helsinki); M. Weber (CCNY);
Phone: (FTS)-666-3710 or (516)-282-3710

$ 630,000 02-2

Investigations of perfect and imperfect solids and their surfaces by newly developed experimental methods; use of both magnetically and electrostatically focussed variable energy positron beams coupled with standard surface analysis tools (Auger Electron Spectroscopy, Low Energy Electron Diffraction, Photoemission, Thermal Desorption Spectroscopy); high resolution positron energy loss measurements of adsorbed molecules on metal surfaces, surface state lifetimes, positron diffusion lengths, positron work functions, positronium formation with measurement of its emitted energy distribution, metal-metal and metal-insulator interface and ion implanted and laser annealed semiconductors; use of recently developed μSR channel at AGS.

64. EXPERIMENTAL RESEARCH - ADVANCED MATERIALS SYNTHESIS AND CHARACTERIZATION

D. E. Cox, A. Moodenbaugh
Phone: (FTS) 666-3818/3870 or (516)-282-3818/3870

$ 365,000 02-2

Preparation and characterization of inorganic materials by high temperature, sputtering and solution techniques, crystal orientation; development and application of profile methods for structural analysis of neutron and x-ray powder diffraction data; application of synchrotron radiation to high resolution powder diffractometry.

BROOKHAVEN NATIONAL LABORATORY (continued)

65. THEORETICAL RESEARCH
V. J. Emery, P. Bak, R. Bruinsma, J. Davenport, G. J. Dienes, W. Finger, R. E. Watson, A. Zangwill
Phone: (FTS) 666-3765 or (516)-282-3765

$640,000 02-3

Phase transitions, critical and cooperative phenomena in magnetic systems, organic metals and incommensurate structures; properties of one- and two-dimensional materials by analytic and numerical methods; nonlinear systems; metal surfaces and adsorbed films; electronic structure of metals and alloys; x-ray and neutron scattering; properties of disordered materials and crystal defect physics; high pressure, high temperature properties of solids.

66. PARTICLE-SOLID INTERACTIONS - RADIATION EFFECTS RESEARCH
K. G. Lynn, P. W. Levy, G. L. Snead, Jr. (DAS), K. J. Swyler (DNE)
Phone: (FTS)-666-3710 or (516)-282-3710

$ 320,000 02-4

Experimental studies of radiation-induced defects in high technology crystals in synthetic and natural minerals, in situ measurements of optical absorption and radioluminescence during electron bombardment, thermoluminescence studies in dosimeter crystals, oxides, quartz and other minerals; theory of thermoluminescence kinetics; theory of radiation; damage formation in irradiated nonmetals; radiation effects in metals, alloys and semiconductors studied by positron annihilation techniques; use of 3-MeV electron accelerator for radiation effects research. Studies on radiation damage in rock salt and other minerals encountered in waste repositories. (Supported minimally by BES.)

67. ENGINEERING PHYSICS - SURFACE SPECTROSCOPY
M. Strongin, W. Eberhardt, P. Johnson, V.J. Murgai, S. L. Weng, P. Wesner
Phone: (FTS)-666-3763 or (516)-282-3763

$ 550,000 02-5

Synchroton Radiation as a technique to study the geometrical and electronic properties of surfaces and interfaces; the use of other surface techniques such as LEED and AES, and the development of new spectroscopies such as inverse photoemission and spin polarized photoemission; techniques used to study problems including a) electronic and geometrical properties of surfaces and interfaces with special emphasis on the properties of metal overlayers, b) hydrogen on transition metals, c) organic molecules on surfaces, d) properties of catalytic surfaces, e) cooperative effects and phase transitions in adsorbate layers on surfaces, f) properties of surface compounds, g) properties of ion implanted surfaces, h) the magnetic properties of thin films.

68. LOW TEMPERATURE SURFACE PHYSICS
M. Strongin, P. Johnson, V.J. Murgai
Phone: (FTS)-666-3763 or (516)-282-3763

$ 270,000 02-5

Photoemission in disordered systems; rare gases on metal surfaces; the electronic structure of metallic clusters dispersed in rare gas solids; photoemission studies of the metal to insulator transition in granular systems; chemisorption and reactions at low temperatures; dissociation and energy transfer mechanisms on surfaces and the relationship to electronic properties.

High Flux Beam Reactor -02-

G. C. Kinne: (FTS) 666-4061 or 516-282-4061

69. EXPERIMENTAL RESEARCH-HIGH FLUX BEAM REACTOR - OPERATIONS (also see page 158)
G. C. Kinne, D. C. Rorer, M. H. Brooks, R. C. Karol, D. G. Pitcher, M. Zukas, S. Protter, L. Junker, P. Tichler, J. Detweiler, W. Brynda
Phone: (FTS)-666-4061 or (516)-282-4061

$6,300,000 02-1

Operation of the High Flux Beam Reactor, including routine operation and maintenance of the reactor, procurement of the fuel, training of operators, operation and maintenance of a liquid hydrogen moderated cold neutron source, and irradiation of samples for activation analysis, isotope productions and radiation damage studies. Technical assistance is provided for experimental users, especially with regard to radiation shielding and safety review of proposed experiments. Additionally, planning and engineering assistance is provided for projects for upgrading the reactor.

BROOKHAVEN NATIONAL LABORATORY (continued)

National Synchrotron Light Source -02-

J. P. McTague: (FTS) 666-4966 or (516) 282-4966

70. EXPERIMENTAL RESEARCH - NATIONAL SYNCHROTRON LIGHT SOURCE, OPERATIONS AND DEVELOPMENT (also see page 156)
J. McTague, A. van Steenbergen, K. Batchelor, J. Galayda, J. Godel,
J. Hastings, M. Howells, H. Hsieh, R. Klaffky, S. Krinsky, A. Luccio,
C. Pellegrini, W. Thomlinson, G. Williams
Phone: (FTS) 666-4966 or (516) 282-4966
$5,900,000 02-2

The objective of this program is to support operations and development of the National Synchrotron Light Source (NSLS). The operations aspect covers operation and maintenance of the two NSLS electron storage rings and its associated injector combination of linear accelerator-booster synchrotron; operation and maintenance of the photon beam lines of the vacuum ultraviolet (VUV) and X-ray storage rings; and the technical support of experimental users. The development of the NSLS encompasses the further improvement of the storage rings to achieve maximum brightness photon sources and the further development of the photon lines of the facility by means of new developments in high resolution photon optics, state of the art monochromators, X-ray mirror systems, detectors, and so on. The NSLS storage rings will provide extremely bright photon sources, several orders of magnitude more intense in the VUV and X-ray regions than conventional sources. While the original design has been solidly based on well developed principles of accelerator technology, this facility is the first in this country to be designed expressly for use of synchrotron radiation, and the objectives in machine performance are quite different from those of importance in high energy physics applications. An extensive R&D program is therefore necessary in order to optimize performance characteristics and also to develop new beam line instrumentation which will permit users to take full advantage of the unique research capabilities to be offered by this important new facility.

IDAHO NATIONAL ENGINEERING LABORATORY
550 2nd Street
Idaho Falls, ID 83401

Materials Science Division - 01

D. D. Keiser - Phone (FTS) 583-1770 or (208) 526-1770

71. MATERIALS SCIENCE WELDING RESEARCH
J. F. Key, H. B. Smartt, G. R. Smolik, J. W. Chan
Phone: (208)-526-8332

$400,000 01-5

Heat source/molten pool interaction studies utilizing high-speed cinematography, optical emission spectroscopy, holography, and infrared thermography to develop process models. Process parameter, material properties, solidification structure relationships. Optical metallographic microstructure characterization; solidification and heat flow modeling.

ILLINOIS, UNIVERSITY OF
at Urbana-Champaign
Urbana, Illinois 61801

Materials Research Laboratory
C. P. Flynn - Phone: (217)-333-1370

72. EFFECT OF FLUID FLOW ON LOCALIZED CORROSION
R. C. Alkire
Phone: (217)-333-0063
$ 70,000 01-1

Transport, kinetics and convective diffusion at localized corrosion sites. Erosion, cavitation, pitting, repassivation, and transient metal salt films.

73. CENTER FOR MICROANALYSIS OF MATERIALS (also see page 174)
H. K. Birnbaum, J. A. Eades
Phone: (217)-333-8396
$210,000 01-1

Chemical, physical and structural characterization of materials. Surface and bulk microanalysis. Electron microscopy, x-ray diffraction, Auger spectroscopy, SIMS and other techniques. Collaborative research programs.

74. RAPID SOLIDIFICATION PROCESSING
H. L. Fraser
Phone: (217)-333-1975
$170,000 01-1

Development of rapid solidification processing of alloys with powder preparation by laser, spin and centrifugal atomization and subsequent consolidation by dynamic compaction techniques. Characterization of microstructure and measurement of properties developed by heat treatments.

75. SEMICONDUCTOR CRYSTAL GROWTH BY ION BEAM SPUTTERING
J. E. Greene
Phone: (217)-333-0747
$150,000 01-1

Mechanisms and kinetics of crystal growth. Metastable single crystal alloys for solar and optical applications. Ion beam sputtering, molecular beam epitaxy, laser heating and low energy ion bombardment methods applied to III-V based compounds and II-IV-V_2 chalcopyrite systems.

76. GRAIN GROWTH IN ALUMINA
D. S. Phillips
Phone: (217)-333-6440
$ 80,000 01-1

Transmission and analytical electron microscopy; characterization of grain boundaries in solid-state and liquid-phase sintered aluminas. Correlation of boundary mobilities in annealed thin films with these microstructures.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

77. LASER PROCESSING OF MATERIALS SURFACES
J. M. Rigsbee and S. H. Risbud
Phone: (217)-333-6584
$ 50,000 01-1

Laser processing to modify structure, composition and physical properties of metallic and ceramic surfaces. Erosion and abrasion resistant surfaces.

78. MICROCHEMISTRY OF SOLIDS
C. W. Wert
Phone: (217)-333-1440
$ 60,000 01-1

Examination of sulfides and clays in coal by electron microscopy. Visco-elastic properties of coal and oil shale for characterization of polymer-like macromolecular nature of carbonaceous matter.

79. HYDROGEN BEHAVIOR IN BCC METALS
H. K. Birnbaum
Phone: (217)-333-1901
$190,000 01-2

Hydrogen, deuterium, tritium and helium mobility in niobium, tantalum, vanadium and nickel through classical and quantum mobility regimes. Properties and phase transitions of group Vb metal hydrides; neutron, surface, permeation and anelastic techniques. Mechanisms of hydrogen transfer across solid interfaces.

80. COUNCIL ON MATERIALS SCIENCE
D. Lazarus
Phone: (217)-333-0492
$ 60,000 01-2

Study and analysis of current and proposed basic research programs on materials and assessment of their relevance to problems of energy utilization. Consideration of national facilities needs. Convening of panel studies on selected topics.

81. STRUCTURE, CRACKING AND CORROSION OF CERAMIC GRAIN BOUNDARIES
S. D. Brown, W. T. Petuskey, A. Zangvil
Phone: (217)-333-4766
$ 60,000 01-2

Effects of impurities on structure and chemistry of regions contiguous to grain boundaries in SiC and Si_3N_4. Delayed failure, fracture toughness, creep and corrosion. Emphasis on effects of partial presures of hydrogen on strength properties. Structure of AlN-SiC solid solutions.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

82. PHYSICAL PROPERTIES OF CERAMIC MATERIALS
W. S. Williams
Phone: (217)-333-3524
$ 95,000 01-2

Flow stress of diborides and non-stoichiometric monocarbides of IVb and Vb transition metals at extremely high temperatures. Dislocation properties, second phase precipitates, and their role in diffusion limitation on flow stress. Microchemical analysis by EELS.

83. OXYGEN IN REFRACTORY BCC METALS
C. J. Altstetter
Phone: (217)-333-4985
$ 65,000 01-3

Thermodynamics and diffusion of oxygen in BCC refractory metals and dilute and concentrated alloys using solid electrolyte cells. Testing of statistical mechanical models relating diffusion and thermodynamic behavior.

84. DEVITRIFICATION BEHAVIOR IN METAL-CONTAINING SILICATE AND BOROSILICATE GLASSES
H. Chen
Phone: (217)-333-7636
$ 90,000 01-3

EXAFS, small and wide angle x-ray scattering and SEM investigation of devitrification kinetics and associated microstructural and compositional changes in silicate and borosilicate based glasses containing metal oxides.

85. DIELECTRIC SOLIDS
D. A. Payne
Phone: (217)-333-2937
$110,000 01-3

STEM, Auger and SIMS analysis of boundary conditions in electrical and structural ceramics, flux growth of ferroelectric crystals; powder preparation by molten salt synthesis and hydrothermal methods. Dielectrophoretic alignment of particles, hot-forging and hot-extrusion of ceramics; electrodes for the photoassisted electrolysis of water.

86. TRAPPING OF HYDROGEN BY SUBSTITUTIONAL SOLUTES IN REFRACTORY METAL ALLOYS
T. J. Rowland
Phone: (217)-333-1726
$ 45,000 01-3

Solute-host bonding and hydrogen distribution in refractory metal alloys containing H in solution; temperature dependence; inelastic neutron scattering, nuclear magnetic resonance, EXAFS, resistivity studies.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

87. MICROWAVE STUDIES OF DISORDERED MATERIALS
H. J. Stapleton
Phone: (217)-333-0073
$100,000 01-3

Effects of tunnelling states and disorder in amorphous semiconductors, fast ionic conductors, and doped crystals using electron spin relaxation, ER, ENDOR, and microwave dielectric susceptibility in the 0.25-25 K range.

88. LOW TEMPERATURE STUDIES OF DEFECTS IN SOLIDS
A. C. Anderson
Phone: (217)-333-2866
$ 90,000 02-2

Experimental studies of glassy metals, of fast ion conductors, of polymers, composites and ceramics, and of irradiated or deformed ionic and other crystals; influence of defects and disorder on macroscopic properties including specific heat, magnetic susceptibility, thermal and electrical transport, thermal expansion, and ultrasonic and dielectric dispersion at 0.02-200K.

89. PHOTOEMISSION STUDIES OF THE ELECTRONIC STRUCTURE OF SURFACES AND INTERFACES
T.-C. Chiang
Phone: (217)-333-2593
$110,000 02-2

Synchrotron radiation photoemission studies of electronic structure of metal surfaces, semiconductor surfaces and interfaces prepared in-situ by molecular beam epitaxy; adsorption kinetics and catalysis on surfaces.

90. RESPONSE OF SOLIDS TO ELECTROMAGNETIC RADIATION
J. D. Dow
Phone: (217)-333-2891 $100,000 02-2

Theory of synchrotron radiation spectra of deep cores in metals and semiconductors. Theory of semiconductor surface states. Theory of surface reconstruction geometries of semiconductors. Theory of disordered systems and alloys.

91. USE OF VERY HIGH PRESURE TO INVESTIGATE THE STRUCTURE OF MATTER
H. G. Drickamer
Phone: (217)-333-0025
$155,000 02-2

High pressure studies of the effect of tuning of energy levels and the change of macroscopic variables on atomic and molecular states and processes in condensed phases, applied to luminescence properties and optical effects at semiconductor-electrolyte interfaces.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

92. EXCITON COLLECTION FROM ANTENNA SYSTEMS INTO ACCESSIBLE TRAPS
L. R. Faulkner
Phone: (217)-333-8306
$ 70,000 02-2

Exciton propagation from absorbing chromophores in polymer films to trapping sites on film surfaces at monolayer coverage. Controlled molecular assemblies of three dimensional reaction systems.

93. FOREIGN ATOMS IN SUPERCONDUCTORS
D. M. Ginsberg
Phone: (217)-333-4356
$ 60,000 02-2

Use of tunnelling and critical field measurements to investigate the effect of magnetic impurities on the electronic and dynamical properties of superconductors.

94. ULTRASONIC STUDIES OF THE STRUCTURE OF MATTER
A. V. Granato
Phone: (217)-333-2639
$130,000 02-2

Investigation by ultrasonic methods of impurity - self interstitial interactions in electron irradiated metals and semiconductors, and of hydrogen in bcc metals.

95. DEFECT AND ELECTRONIC PROPERTIES OF SOLIDS
D. Lazarus
Phone: (217)-333-0492
$ 60,000 02-2

Atomic mobility and electrical conduction in solid electrolytes and metallic glasses, studied as a function of temperature and pressure. Mainly concerned with elucidating atomistic defect formation and jump processes.

96. PROPERTIES OF CRYSTALLINE CONDENSED GASES
R. O. Simmons, V. R. Pandharipande
Phone: (217)-333-3760
$160,000 02-2

Measurement and theory of momentum density in bcc, hcp, and liquid helium; pulsed neutron scattering; phase transitions and structure determination in solid hydrogen by neutron diffraction; isotopic phase separation in solid helium; thermal and isotopic defects in helium crystals; quantum effects in diffusion.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

97. NUCLEAR MAGNETIC RESONANCE IN SOLIDS
C. P. Slichter
Phone: (217)-333-3834
$155,000 02-2

Investigations of layered materials and one dimensional conductors with charge density waves, of platinum-alumina reforming hydrocarbon catalysts, and of spin glasses using nuclear magnetic resonance methods.

98. PHYSICAL PROPERTIES OF ORDERED AND DISORDERED SOLID SOLUTIONS
H. Zabel $120,000 02-2

Phone: (217)-333-2514

X-ray and neutron scattering investigations of structural, thermal and vibrational properties of alkali metal graphite-intercalation compounds; staging, dislocation and point defects, phonon dispersion, and order-disorder transformations.

LAWRENCE BERKELEY LABORATORY
University of California
Berkeley, California 94720

Materials and Molecular Research Division

A. W. Searcy - Phone: (FTS) 451-6062, or 415/486-6062

99. Structure and Properties of Transformation Interfaces
R. Gronsky
Phone: (415) 486-5674, or FTS 451-5674
160,000 01-1

Characterization of the structure and composition of interfaces at high spatial resolution: grain boundaries, interphase boundaries, and free surfaces. Determination of the role of interfaces in solid-state reactions: structural and compositional evolution accompanying transformations.

100. Microstructure, Properties, Alloy Design: Inorganic Materials
G. Thomas
Phone: (415) 486-5656, or FTS 451-5656
540,000 01-1

Relationships between microstructure and properties; control of properties through characterization and control of structure; application of principles of strengthening and phase transformations to alloy design for mechanical (including wear) and magnetic property improvements--energy conservation; systems under investigation include ferrous alloys, dual-phase steels, rare-earth and Co-free alloys, and ceramics. Quantitative analyses of structure by electron microscopy, spectroscopy and diffraction, and high voltage, high resolution electron microscopy.

101. Solid State Phase Transformation Mechanisms
K. H. Westmacott
Phone: (415) 486-5663, or FTS 451-5663
180,000 01-1

Mechanisms of phase transformation are studied using a variety of transmission electron microscopy techniques. Specifically, the role of crystal lattice defects in precipitation reactions, vacancy-solute atom interactions in substitutional and interstitial alloy systems, segregation phenomena, impurity and minor alloy addition effects. Interrelationships between precipitation sequence, habit plane, interface structure, and orientation relations are being established for different crystal structures and compared with a developing crystallographic theory.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

102. National Center for Electron Microscopy (also see page 168)
G. Thomas, R. Gronsky, and K. H. Westmacott
Phones: (415) 486-5656, or FTS 451-5656;
(415) 486-5674, or FTS 451-5674;
(415) 486-5663, or FTS 451-5663
880,000 01-1

Organization and operation of a collaborative research resource for transmission electron microscopy. Maintenance, development, and application of specialized instrumentation, including an Atomic Resolution Microscope (ARM) for ultrahigh resolution imaging; a 1.5 MeV High Voltage Electron Microscope (HVEM) with capabilities for dynamic in-situ observations; analytical electron microscopes for microchemical analysis; and support facilities for specimen preparation, imaging analysis, image simulation, and instrument development.

103. In-Situ Investigations of Gas-Solid Reactions by Electron Microscopy
J. W. Evans and K. H. Westmacott
Phones: (415) 642-3807;
(415) 486-5663, or FTS 451-5663
100,000 01-1

The investigation of reactions using an environmental cell in the 650 kV and 1.5 MeV high voltage electron microscopes. Emphasis is on investigation of the effect of microstructure, e.g., grain boundaries, microcracks, on the reactions between gases and solids. In-situ reductions of Fe_3O_4 to FeO by hydrogen-argon mixtures have been carried out and precipitates of FeO identified by electron diffraction and lattice fringe imaging. Characterization of commercial Fe and Cr containing oxide refractories by high voltage microscopy and energy dispersive X-ray/SEM is being performed together with in-situ reduction experiments.

104. Local Atomic Configurations in Solid Solutions
D. de Fontaine
Phone: (415) 642-8177
80,000 01-1

Study of the early stages of phase transformations in materials, primarily metallic alloys. A strong theoretical component dealing with detailed calculations of local atomic arrangements characteristic of incipient ordering and clustering. Atomic ordering studied in systems exhibiting the phenomenon of long-period superstructure formation, the theoretical tool being the cluster variation method of statistical thermodynamics and low-temperature expansion of the exact free energy, the experimental tool being high-resolution electron microscopy. Clustering, i.e., phase separation, to be studied in systems exhibiting partitioning of substitutional and interstitial alloying elements, such as alloy steels, the theoretical tool here being multicomponent nucleation theory and the experimental tool being transmission electron microscopy with full analytical capabilities.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

105. Collaborative Studies by TEM
A. W. Searcy
Phone: (415) 486-6062, or FTS 451-6062
40,000 01-1

Increased utilization of unique TEM instrumentation is promoted by interdisciplinary collaborations between nonelectron microscropist Divisional scientists and resident or visiting TEM specialists. Advanced high resolution, high voltage, and microanalytical techniques are applied to a variety of important scientific questions. Current studies include relationship between properties and rate of graphitization in carbon blacks, structural characterization of the graphite intercalation compound, $C_{2.0}F$, and short-range-order in Au_4Fe and its relation to magnetic properties.

106. Theoretical Problems in Alloy Design
J. W. Morris, Jr.
Phone: (415) 486-6482, or FTS 451-6482;
(415) 642-3815
505,000 01-2

The project has three objectives: to build the scientific foundation needed to approach the problem of alloy design in a systematic way, to develop systematic approaches, and to create new alloys that satisfy advanced energy needs. Specific research tasks include: (1) theory of phase transformations in solids and influence of microstructure on engineering properties; (2) experimental research on fundamental problems in metallurgy, including the control of microstructure through thermomechanical processing, the influence of microstructure on engineering properties, and the development of probative materials testing techniques, (3) the development of new structural alloys for advanced energy systems, now mainly concerned with the design of improved structural alloys for low-temperature use; (4) welding metallurgy, including the development of appropriate weld filler metals and weld microstructures to maintain toughness in high strength welded alloys; (5) the development of improved superconducting wires for use in high field superconducting magnets.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

107. Mechanical Properties of Ceramics
A. G. Evans
Phone: (415) 642-7347
280,000 01-2

This project is concerned with the mechanical reliability of ceramics at high temperatures. The principal research emphases are the development of a predictive capability for high temperature failure and for microstructure development during final stage sintering. Elevated temperature failure studies are concerned with the evolution of cavities and cracks at grain boundaries and within second phases. Experimental cavitation measurements are correlated with theoretical models containing the dominant microstructural variables. Final stage sintering studies are examining the processes that dictate exaggerated grain growth, retained porosity and the coarsening of the general microstructure. Theoretical descriptions are compared with microstructural measurements.

108. Environmentally Affected Crack Growth in Engineering Materials
R. O. Ritchie
Phones: (415) 486-5544, or FTS 451-5544;
(415) 642-0417
190,000 01-2

The role of microstructure and environment in influencing the subcritical and critical propagation of cracks in ferrous alloys is being examined with specific reference to i) fatigue crack growth behavior at ultralow near-threshold growth rates ($<10^{-9}$ m/cycle), ii) crack extension behavior of short flaws (comparable in size to the scale of microstructure or scale of local plasticity), and iii) the micromechanics of transgranular cleavage fracture. Research on near-threshold and short crack fatigue crack growth has been directed towards identifying mechanisms of crack closure and their role in influencing behavior. Specifically mechanisms involving cyclic plasticity, corrosion debris, meandering crack paths, viscous fluids and metallurgical phase transformations have been examined and modelled based on experimental results or bainitic, duplex ferritic/martensitic, and austenite steels.

109. High-Temperature Reactions
A. W. Searcy
Phone: 415/486-6062, or FTS 451-6062
295,000 01-3

Thermodynamics and kinetics of decomposition reactions. Thermodynamics theory for surfaces, particle shapes, and heterogeneous equilibria. Surface diffusion of vapors through porous solids. Experimental and theoretical studies of adsorption. Sintering of submicron particles. Thermodynamics of highly non-ideal carbonate solutions.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

110. Structure-Property Relationships in Semiconductor Materials
J. Washburn
Phone: (415) 486-6254, or FTS 451-6254
310,000 01-3

Structure sensitive electrical properties of semiconductor materials. Topics with close relation to state-of-the-art technology investigated jointly with the semiconductor industry and with Electrical Engineering and Computer Sciences Department at Berkeley. Use of unique high-voltage and high-resolution electron microscope facilities at Lawrence Berkeley Laboratory for the characterization of interfaces, precipitates, dislocation substructures, and radiation-induced damage. These facilities and the Rutherford scattering facility are currently being utilized for a systematic study of the crystal-to-amorphous transformation in silicon and gallium arsenide during ion implantation and to the effect of impurities and dopant elements on the kinetics of crystal growth into amorphous zones. High-resolution electron microscopy is also providing detailed information concerning the mechanisms of formation and degradation of the Cu_2S layer in $CdS-Su_2S$ solar cells.

111. Properties and Processing of Refractory Ceramics
L. C. De Jonghe
Phone: (415) 486-6138, or FTS 451-6138
235,000 01-3

Mechanisms and kinetics of the reduction of mixed oxides by hydrogen or CO/CO_2 and study of these reactions by thermogravimetry and microanalytical and electron-optical methods. Densification and reaction in Al_2O_3-CaO powder mixtures; modeling and experiments on multiparticle sintering; densification with loading. Liquid phase and transient liquid phase densification. Rearrangement processes during sintering.

112. Structure and Electrical Properties of Composite Materials
R. H. Bragg
Phone: (415) 642-7393
125,000 01-3

Structure, electronic, and thermophysical properties of carbon materials heat treated in the range of 1000°C-3000°C. Characterization using X-ray and neutron scattering, and magnetic susceptibility, thermoelectron power, internal friction, gas permeability, C^{13} and H^1 nuclear magnetic resonance (NMR), secondary ion mass spectroscopy (SIMS), and thermogravimeter analysis (TGA) measurements.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

113. High-Temperature Oxidation and Corrosion of Materials
A. W. Searcy
Phone: (415) 486-6062, or FTS 451-6062
315,000 01-3

Mechanisms and kinetics of high-temperature corrosion reactions, in particular: the initial scale development; transport in and through scales; the scale's structure, morphology and growth mode; the mechanical integrity and adherence of the scale to the substrate; and the chemical integrity of the scale when exposed to corrosive sulfate deposits. Oxide stoichiometry changes in the presence of sulfur and transport studies in oxide solutions and their relationships to mechanisms of degradation. Active element additions to alloys and coatings to promote scale/substrate adhesion. Studies are based on thermogravimetric analyses and microscope techniques, including scanning Auger analysis.

114. Ceramic Interfaces
A. M. Glaeser
Phone: (415) 642-3821
105,000 01-3

Investigation of grain boundary migration behavior and its effects on microstructure development and stability in high-temperature oxide ceramics. Development and refinement of experimental techniques permitting the influence of solutes, pores, etc., on grain boundary migration rates to be isolated and systematically investigated. Synthesis, characterization and processing of doped and undoped alumina powders; fabrication of alumina ceramics having controlled composition and microstructure. Determination of the influence of MgO content, driving force, and temperature on migration behavior of individual grain boundaries in Al_2O_3. Experimental investigation of boundary structure transformations and their influence on microstructure development.

115. Abrasive, Erosive, and Sliding Wear of Materials
I. Finnie
Phone: (415) 642-1496
120,000 01-5

Mechanisms of abrasive, erosive and sliding wear. Simulation of microscopic wear processes by larger scale tests. Study of the effect of particle size, shape and hardness to abrasive and erosive wear. The influence of temperature and materials properties on wear rates. Correlation of wear rates to mechanical properties.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

116. Erosion of Brittle Solids
A. G. Evans
Phone: (415) 642-7347
110,000 01-5

This project is concerned with the development of a fundamental understanding of erosion and strength degradation in brittle layers and coatings subject to impact by solid particles. The principle research directions involve studies both of the damage created by the impact and indentation of individual particles and of the erosion characteristics under multiple impact conditions. The studies emphasize the influence of residual stress on the buckling and spalling of thin surface layers. The mechanics of buckling are being studied and related to crack driving forces. Relations between residual stress and spalling provide the basis for interpreting erosion data on these systems.

117. Far-Infrared Spectroscopy
P. L. Richards
Phone: (415) 642-3027
220,000 02-2

Development of improved types of far infrared detectors, mixers and spectrometers. Use of advanced infrared techniques for the measurement of: the vibrational frequencies of molecules chemically bound to metal surfaces, the infrared properties of solids with charge-density wave transitions, the far infrared spectra of organic superconductors, and the infrared photoconductivity of impurities in semiconductors.

118. Experimental Solid-State Physics and Quantum Electronics
Y. R. Shen
Phone: (415) 642-4856
255,000 02-2

The main objective of this program is to further the understanding of lasers and laser-related physics. Emphasis is on the development of linear and nonlinear optical techniques for material studies. They are being used to study current problems of interest: isotope separation, photochemistry, surface physics, and phase transitions. Recent concerted effort is in surface second harmonic generation. It is being developed to probe adsorbates at surfaces and interfaces, even between two condensed media. Theoretical and experimental investigation on various aspects of nonlinear optical interactionn with surfaces is being carried out.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

119. Excitation in Solids
C. D. Jeffries
Phone: (415) 642-3382

	162,000	02-2

Study of phenomena arising when light strikes matter, in particular semiconductors like germanium: electrons are excited, leaving vacant states, or holes. At sufficient densities, excitons condense into a metallic electron-hole liquid, a novel state of matter. An unusual period doubling leading to noisy chaotic behavior is observed, which can be understood in terms of a recent universal model of approach to chaos by period doubling bifurcations. To verify this, a driven nonlinear semiconductor oscillator is being studies experimentally for a wide class of nonlinear phenomena in solids, to test the validity of universal models of routes to chaos.

120. Time-Resolved Spectroscopies in Solids
P. Y. Yu
Phone: (415) 642-8087

	69,000	02-2

Application of an optical system capable of measuring adsorptivity, reflectivity, photoluminescence and light scattering spectra with time resolution of picoseconds to the study of the following phenomena: relaxation of photoexcited hot carriers via carrier-phonon interaction; decay of nonequilibrium phonon populations; temperal behavior of resonant Raman spectra and hot luminescence; trapping of carriers by deep impurity levels in semiconductors and propagation of short pulses through dispersive media.

121. Superconductivity, Superconducting Devices, and 1/f Noise
J. Clarke
Phone: (415) 642-3069

	274,000	02-2

Development of Superconducting Quantum Interference Devices (SQUIDs) for measuring voltage and fluctuations in magnetic fields and magnetic field gradients, quantum noise processes in Josephson junctions and SQUIDS, operation of SQUIDs as high-frequency amplifiers. use of SQUIDs in magnetotelluric measurements of the apparent resistivity of the earth's crust, use of SQUIDS to measure magnetic field gradient fluctuations at the earth's surface. Chaos and noise in Josephson circuits. Investigation of thermoelectric effects in superconductors. Measurement of electron-phonon relaxation times in superconductors. Study of 1/f noise in Josephson junctions and SQUIDs. Dependence of 1/f noise in metal films on material properties.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

122. Theoretical Studies of the Electronic Properties of Solid Surfaces
L. M. Falicov
Phone: (415) 642-5993
70,000 02-3

Theoretical studies of: (a) the structural properties of surfaces, namely, the organization and arrangement of atomic constituents at equilibrium; (b) the constitutional properties of the surface, in particular the segregation properties of alloys at the surface as a function of crystal structure, surface orientation, nominal chemical composition, and temperature; (c) the electronic structure of surfaces, in particular electron states and electron densities in the neighborhood of the surface; (d) the vibronic properties of surfaces; (e) the magnetic properties of surfaces, both in magnetic solids (ferromagnetic and antiferromagnetic) or in nonmagnetic solids which may develop a magnetic surface layer; (f) the chemical--in particular the catalytic--properties of solids as they are related to the basic physical properties (a)-(e).

123. Theoretical Solid-State Physics
M. L. Cohen
Phone: (415) 642-4753
100,000 02-3

A first-principle quantum mechanical approach is used to explain and predict properties of solids. The specific techniques involve the use of pseudopotentials for electron-ion interactions, the local-density approximation for electron-electron interactions, and a momentum space total energy technique for computing structural properties. Applications to many areas in condensed matter science are made. These include: surfaces and interfaces, chemisorption, electronic band structure, optical reflectivity and photoemission, superconductivity, vibrational and structural properties, and solid-solid phase transitions.

124. Low-Temperature Properties of Materials
N. E. Phillips
Phone: (415) 642-4855
140,000 03-1

The general objective of this program is to obtain low-temperature data, particularly heat-capacity data, that contribute to an understanding of the relations between atomic properties and the macroscopic properties of materials. The materials investigated include normal and superconducting metals, superfluids, dielectric solids, and magnetic materials. Heat capacity measurements are confined to temperatures below 25 K because usually only in that region can the various contributions be reliably separated. The temperature scale for the region from 0.06 to 25 K is maintained on germanium thermometers and its relation to various "absolute" scales is well established. For temperatures from 0.06 K to the mK region, γ-ray anisotropy and nuclear susceptibility thermometers are used as primary thermometers, and various magnetic thermometers are used as working thermometers.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

125. Electrochemical Processes
C. W. Tobias
Phone: (415) 486-5208, or FTS 451-5208;
(415) 642-3764
130,000 03-1

This program is designed to advance the scientific foundations of electrochemical engineering, and to widen the range of useful applications of electrochemical transformations. Mass and charge transport in cell processes: combined influences of electrode geometry, surface potential, and ionic transport on the distribution of current on electrode profiles. Characterization of novel methods for reducing mass transfer resistance in high rate applications. Nonaqueous ionizing solvents: thermodynamic and kinetic properties of electrode reactions which are not feasible in aqueous media.

126. High-Temperature Thermodynamics
L. Brewer
Phone: (415) 486-5946, or FTS 451-5946
149,000 03-3

Characterization of the high-temperature chemical behavior of materials, particularly refractory ceramic materials, metals, and gases. The high-temperature thermodynamic properties are being determined through use of solid-electrochemical cells, solid-gas equilibria, and by X-ray and metallographic characterization of phase boundaries. The data are being used to test and improve chemical models capable of predicting the thermodynamic and elastic properties of high-temperature materials.

127. Chemistry and Materials Problems in Energy Production Technologies
D. R. Olander
Phone: (415) 642-7055
256,000 03-3

Investigation of the chemical and physical behavior of materials in the environments characteristic of energy production devices, with major emphasis on fission and fusion reactors. Experiment and study of the mechanisms involved in the high temperature behavior of uranium fuel compounds and Zircaloy cladding: transient vaporization, surface self-diffusion, high temperature corrosion and hydrogen solubility; volatile fission product release from irradiated UO_2. Molecular beam studies of chemical kinetics include hydrogen atom reaction with ceramic oxides and refractory carbides and the reactions of halogens with metals, both solid and liquid.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

128. Plasma-Enhanced Deposition of Thin Films
D. W. Hess
Phone: (415) 642-4862
49,000 03-3

This program is designed to establish scientific foundations for the rf plasma-enhanced deposition of thin films; control of chemical, magnetic, optical and electrical properties by variation of deposition parameters. Kinetic models of deposition processes as they affect solar cell fabrication, integrated circuit processing, magnetic film properties, and structure-property relations in catalyst support materials.

129. Electrochemical Phase Boundaries
R. H. Muller
Phone: (415) 486-6079, or FTS 451-6079
172,000 03-3

Advancement of the understanding of thin films and boundary layers at solid-liquid interfaces. Development and use of optical techniques for the observation of surfaces. Composition, structure and transformation of thin films, effect on chemical properties of metals and on metal deposition and dissolution reactions. Structure of adsorbed monolayers and their use for the control of phase-nucleation and growth in electrocrystallization. Determination of multilayer film structures by use of a unique self-compensating spectroscopic ellipsometer and its combination with electron spectroscopy. Investigation of boundary layers by optical interferometry; new methods to accelerate electrochemical mass transfer; control of high-rate electrolytic processes. Surface forces and thin-film interference in electrolyte films on metals.

130. Solid-State and Surface Reactions
G. A. Somorjai
Phone: (415) 642-4053; (415) 486-6160, or FTS 451-6160
(415) 486-6067, or FTS 451-6067
362,000 03-3

The research program is centered on studies of catalyzed surface reaction investigations of the atomic structure and chemical composition of solid surfaces and adsorbed monolayers. The kinetics and mechanisms of catalytic surface reactions are studied using well-characterized crystal surfaces at low and high pressures by using a combination of surface science techniques. The materials that are the focus of our studies are platinum, rhodium, iron and its compounds, rhenium, molybdenum, alkali metals and bimetallic alloys. The adsorbates and reactants are mostly hydrocarbons, oxygen, hydrogen and water. Part of the investigation is directed toward the atomic the atomic scale understanding of the structure and catalytic behavior of metal surfaces. The other part of the studies is aimed at developing new catalysts which substitute for precious metals and exhibit high rates and selectivity.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division -01- (Continued)

131. Nuclear Magnetic Resonance
A. Pines
Phones: (415) 486-6097, or FTS 451-6097;
(415) 642-1220
162,000 03-3

The primary objectives of the nuclear magnetism program are to develop methods in magnetic resonance spectroscopy and to use them to study molecular behavior in condensed phases. This demands an understanding of the interaction of nuclear spins with each other, with other degrees of freedom such as molecular translations, vibrations and rotations, and with external radiation such as light or radiofrequency sources. Novel methods developed under the program include multiple quantum spectroscopy, high resolution solid state NMR and magic angle spinning, zero field NMR, pulsed laser nuclear double resonance and nuclear magnetic isotope separation. These methods are being applied to understand structure and dynamics at the molecular level in a number of materials including ferroelectrics, liquid crystals, polymers, organic crystals and zeolites. Some molecular properties change upon light excitation, and laser magnetic double resonance is being used to examine how these changes dictate the course of photochemical reactions.

132. Erosion-Corrosion Wear
A. V. Levy
Phone: (415) 486-5822, or FTS 451-5822
100,000 01-5

The combined model for prediction of erosion of ductile metals will be developed and experimentally verified. The model, developed from analytical expressions that define the two-phase fluid flow of a gas-solid particle stream and equations that describe the platelet mechanism of erosion, will be refined in accordance with test data. The flow test data will be generated using the LDV instrumented flow system to define the velocity, impact angle, particle size distribution, and solids loading of stream flow in various piping system geometries. The erosion data will be obtained using representative alloys used in coal conversion and combustion systems. The use of boundary layer gas to protect the surface of coal reactors from high-temperature corrosion that has analytically been proven to be feasible will be experimentally studied.

LAWRENCE LIVERMORE NATIONAL LABORATORY
P. O. Box 808
Livermore, California 94550

Materials Science Division - 01-

C. F. Cline - Phone (FTS) 532-8021 or 415-422-8021

133. HOT CORROSION STUDIES RELATED TO FOSSIL FUELS
J. J. Truhan, O. H. Krikorian
Phone: (FTS) 532-6925

$200,000 01-1

Study of mechanisms and kinetics of hot gas and molten salt corrosion of Ni- and Fe-based alloys; emphasis on reduction of the strategic element Cr in alloys without loss of corrosion resistance; corrosion analysis by thermogravimetric, linear polarization, laser raman spectroscopy, and electron microprobe techniques; alloys studied include Ni-Cr binary and Ni-Cr with separate active element additions of Hf, Ti, Y, and Nb; development of quantitative model relating Cr content to susceptibility of Ni-based alloys to corrosive media at 500-1000 C; development of mechanisms for early and middle stages of corrosion by oxidizing and sulfidizing gases and by molten salts.

134. RAPIDLY QUENCHED ALUMINUM ALLOYS
L. Tanner, L. Jacobsen
Phone: (FTS) 533-2653

$350,000 01-3

Preparation of rapidly quenched metallic alloys based on aluminum characterization and evaluation of prepared alloyws for thermal, mechanical, and corrosion resistant properties. Emphasis on high specific strength and corrosion resistance; examination of aging behavior and detailed phase relationships.

135. OPTICAL MATERIALS RESEARCH
M. J. Weber
Phone: (FTS) 532-5486

$450,000 02-2

Investigation of nonlinear optical properties of transparent materials subject to intense light beams. Intensity-dependent refractive index changes measured using time-resolved laser interferometry. Multiphoton absorption and multiphoton-induced color centers at near-ultraviolet to near-infrared wavelengths detected using photorefractive techniques. Growth and spectroscopy of new laser materials. Laser-induced fluorescence line narrowing and optical site selection spectroscopy to probe variations in local fields and electron-phonon coupling at paramagnetic ion sites in disordered solids. Dependence of spectroscopic and optical properties on materials composition. Materials include oxide and fluoride glasses and crystals.

LAWRENCE LIVERMORE NATIONAL LABORATORY (continued)

136. SURFACE PHYSICS AND CHEMISTRY OF LASER INDUCED DAMAGE

W. J. Siekhaus
Phone: (FTS) 532-6884

$280,000 02-2

Investigation of the fundamental physical and chemical process determining the thresholds for laser-induced damage of transmitting optical materials and thin-film coatings. Studies of the relation between damage thresholds of the bulk and surfaces, dependence of damage thresholds on the physical structure of surfaces, effects of adsorption of foreign atoms, surface chemical reactions, and migration of impurities. Polished crystalline and amorphous samples are cleaned by laser irradiation in a vacuum chamber and tested *in situ* using 1.06, 0.53 and 0.35 m laser pulses. Multiphoton induced electron, neutral atom and ion emission is monitored along with ESCA surface analysis.

137. D-T CRYOGENIC PROPERTIES

P. C. Souers, R. T. Tsugawa and E. M. Fearon
Phone: (FTS) 532-1301

$180,000 03-2

Experimental study of ultraviolet and infrared absorption peaks recently discovered in our laboratory in solid, irradiated hydrogen at temperatures below 8 K. Includes kinetics as a function of temperature and tritium content. Emission studies in the ultraviolet and visible regions also under way. Modeling of ion charge interaction with neutral hydrogen molecules is under way to elucidate the nature of the radiation defects giving rise to the spectra.

LOS ALAMOS NATIONAL LABORATORY
University of California
P. O. Box 1663
Los Alamos, New Mexico 87545

Materials Science and Technology Division

S. S. Hecker - Phone (FTS) 843-4563 or (505)-667-4563

138. THE EFFECT OF SELF-IRRADIATION ON STABILITY OF CERAMIC NUCLEAR WASTE
F. W. Clinard, Jr., G. F. Hurley, D. E. Peterson, D. L. Rohr, R. B. Roof
Phone: (505)-667-5102
$277,000 01-4

Alpha decay self-damage in zirconolite, perovskite, pyrochlore, and multiphase SYNROC ceramic waste; doping with short half-life actinides and examination of natural mineral analogues; role of starting composition and crystal structure; evolution of the metamict state; localized and generalized atomic disorder; alpha recoil tracks; characterization of damage effects by x-ray and electron diffraction, optical and electron microscopy, thermal conductivity, dilatometry, calorimetry, and fractography; swelling, microhardness, fracture toughness, and microcracking; role of elevated temperature during self-damage; post-irradiation annealing and recovery.

139. MECHANICAL PROPERTIES
M. G. Stout, J. J. Petrovic, P. L. Martin
Phone: (505)-667-6750
$360,000 01-5

Response of metals to multiaxial loading and large strains; yield surfaces, multiaxial stress-strain relationships, stress path changes. Characteristics of and mechanisms controlling the large strain deformation of aluminum, nickel, brass; substructural and textural evolution with strain and strain state. Multiaxial loading brittle fracture responses of Al_2O_3, Si_3N_4, SiC, and ZrO_2; Statistical fracture theories for multiaxial loading; mixed-mode fracture of indentation-produced surface flaws and macroscopic cracks; microstructural effects on multiaxial loading brittle fracture.

140. STRUCTURAL CERAMICS
J. J. Petrovic, F. D. Gac, C. Hollabaugh, P. D. Shalek, P. L. Martin
Phone: (505)-667-5452
$226,000 01-5

Studies of fabrication-microstructure-properties interrelationships for structural ceramic materials; synthesis of dense, strong SiC and Si_3N_4 materials without the use of densification additives that can degrade elevated temperature mechanical properties; synthesis of ultrafine/ultrapure SiC and Si_3N_4 powders by RF-plasma methods; activation of powders through shock loading and irradiation treatments; consolidation of powders by colloidal chemistry and hot-pressing methods; relationships between processing and microstructure, mechanical behavior, and oxidation/corrosion response.

LOS ALAMOS NATIONAL LABORATORY (continued)

141. IMPURITY MODIFICATION OF MATERIALS: SURFACE PROPERTIES AND THIN STRUCTURAL FILMS
T. N. Taylor, C. J. Maggiore, R. W. Springer, C. T. Campbell
Phone: (505)-667-4686
$230,000 03-2

Selective modification of chemisorption properties by surface additives; relationship that electronic, structural, and compositional factors have to surface reactivity; vapor deposited metal adatoms on single crystal semimetal or oxide substrates; electron, photoelectron, and thermal desorption spectroscopies, low-energy electron diffraction and work function measurements; crystallographic characterization by MeV ion scattering; structural and mechanical properties of vapor deposited thin film metal/metal-compound laminates; spatial and chemical nature of impurity layers by energetic ion beam analysis and conventional surface sensitive techniques; physical and mechanical properties of vapor deposited films.

Physics Division

J. C. Browne - Phone: (FTS) 843-6162 or (505)-667-6162

142. CONDENSED MATTER RESEARCH WITH THE SNR/PSR FACILITY (also see page 164)
R. N. Silver
Phone: (505)-667-6069
$1,630,000 02-1

Neutron scattering research in condensed matter using the SNR/PSR pulsed spallation neutron source at Los Alamos. Includes studies in most areas of condensed matter; currently metal hydrides, catalysts, liquids, metallic glasses, magnetism, chemical structure, chemical spectroscopy, etc. Development of time-of-flight neutron scattering instrumentation including, currently, a filter difference spectrometer, a liquids and amorphous diffractometer, a powder diffractometer, and an electron volt spectrometer. The SNR/PSR is a national user facility for neutron scattering research in solid state physics, chemistry, materials science, biology, and polymers.

143. ULTRAHIGH-PRESSURE STUDIES OF MOLECULAR CRYSTALS
R. L. Mills, R. A. LeSar
Phone: (505)-667-4129
$200,000 02-5

Study solidification, crystal structures, phase transformations, and thermodynamics of simple dielectrics, hydrides, and polymers from low to high temperature in high-pressure diamond anvil cells (DACs) using UV, IR, and Raman spectroscopy and laser-beam, neutron, and x-ray scattering; develop theories of phase transformation, structural behavior, and chemical reaction kinetics; use DACs to prepare and characterize exotic materials, including rare-gas and hydrogen-containing molecules.

LOS ALAMOS NATIONAL LABORATORY (continued)

144. THERMAL PHYSICS
J. C. Wheatley, G. W. Swift, A. Migliori, M. Maley, (UCSD Students: H. Haucke, J. Helffrich, Y. Maeno, T. Hofler)
Phone: (505)-667-7499
$230,000 02-2

Natural or intrinsically irreversible engines: acoustic engines using liquids and gases, magnetic engines, heat pumps and prime movers; liquid propylene thermodynamic and thermophysical properties; liquid propylene heat engine: regenerators, heat exchangers, mechanicals, seals; thermal convection in dilute solutions of ^{3}He in superfluid ^{4}He near 1 K, steady and oscillatory, nonlinear dynamics, coherence and chaos; spin polarized hydrogen isotopes: transport, thermodynamic properties, magnetosound; normal and superfluid liquid ^{3}He: ferromagnetism, susceptibility anisotropy.

Theoretical Division

G. I. Bell - Phone: (FTS) 843-4401 or (505)-667-4401

145. ELASTIC WAVE SCATTERING AND QUANTITATIVE FLAW AND MICROSTRUCTURE CHARACTERIZATION
R. J. Brind, J. E. Gubernatis, W. M. Visscher
Phone: (505)-667-6727
$180,000 01-5

Development of an analytical scientific reference data base for flaw and microstructure characterization calculations of phenomena selected as representative of applications; integral equation methods, the method of optimized truncation, geometrical diffraction theory and Pade approximations; single scattering results for the flaw characterization studies; multiple scattering theories for the microstructure characterization studies. Investigate use of elastic wave scattering measurements for residual stress evaluation and for characterization of surface cracks.

146. LOS ALAMOS EQUATION OF STATE LIBRARY (also see page 182)
J. Abdallah, B. I. Bennett, F. Dowell, W. F. Huebner, J. D. Johnson, D. Liberman, S. P. Lyon, K. S. Trainor
Phone: (505)-667-5751
$240,000 02-3

Maintain a computer-based library of equations of state (EOS) and other material properties such as opacities, and electrical and thermal conductivities for application to energy and related programs. Survey current user requirements and calculate or acquire and evaluate the needed data. Store data in tabular form suitable for use in realistic hydrodynamic code calculations and other applications. Distribute library programs and data to users on magnetic tapes in a universal computer format. Apply theories of solids, liquids, gases, plasmas, and mixtures to generation of EOS data. Develop new theoretical methods when existing theories and experiments are insufficient to satisfy user requirements.

OAK RIDGE ASSOCIATED UNIVERSITIES
P. O. Box 117
Oak Ridge, Tennessee 37831-0117

A. Wohlpart - Phone (FTS) 626-3421 or (615) 576-3421

147. DOE FACILITY USERS PROGRAM (also see page 172)
A. Wohlpart

$140,000 01-1

Collaborative research between university, industry, and national laboratory scientists in materials sciences to foster access to and use of advanced facilities. The SHaRE (Shared Research Equipment Program) facility includes state-of-the-art capabilities in the areas of transmission and analytical electron microscopy, surface analysis, and nuclear microanalysis; approximately 20% of the usage of these facilities is by SHaRE users for basic and applied research on energy-related materials problems, based on research proposals approved by a review committee. The ORSOAR (Oak Ridge Synchrotron Organization for Advanced Research) program involves the National Synchrotron Light Source at the Brookhaven National Laboratory to study the structures of a wide variety of amorphous and crystalline materials including metallic glasses and liquids containing more than one element, heterogeneous catalysts, surface structures, corrosion films, defects and deformed materials, and local atomic arrangements in metal alloys and ceramics; approximately 40% of the beam time will be allocated to users based on a proposal basis.

OAK RIDGE NATIONAL LABORATORY
P. O. Box X
Oak Ridge, Tennessee 37830

Metals and Ceramics Division -01-

J. R. Weir, Jr. - Phone (FTS) 624-4065 or 615-574-4065
C. J. McHargue - Phone (FTS) 624-4344 or 615-574-4344

148. THEORETICAL STUDIES OF METALS AND ALLOYS
J. S. Faulkner, W. H. Butler, G. S. Painter, G. M. Stocks, D. M. Nicholson
Phone: (615)-574-5161
$550,000 01-1

Local density formalism (LDF) combined with cluster program and layer KKR program to study electronic states of surfaces and energetics such as binding energy of adsorbates, surface molecular dissociation, and chemical properties of reaction intermediates as related to catalysis; small molecular clusters, absorption of O on Al and O, S on Ni; band theory of metals, alloys and compounds, self-consistent KKR-CPA treatment of random substitutional solid solutions, residual resistivity, comparison with results of photoemission experiments, extension of theory beyond CPA; calculation of binding energies and phase stability in alloys; superconducting transition temperature and H_{c_2} and phonon line width; phonon contribution to lattice conduction; electron-phonon and electron-electron enhancement effects in metals; cohesive energy and magnetic moment of Fe.

149. X-RAY SCATTERING RESEARCH
C. J. Sparks, B. S. Borie, G. E. Ice, H. L. Yakel
Phone: (615)-574-6996
$550,000 01-1

Development and use of fluorescence, anomalous dispersion, and scattering techniques for x-rays at the Stanford Synchrotron Radiation Laboratory; design and construction of beam line for installation at the National Synchrotron Light Source, Brookhaven National Laboratory; long- and/or short-range order in Fe-Ni-Cr alloys; atom positions in sigma phase, and alloyed carbides; defects in ion implanted materials; theoretical studies of extinction phenomena.

150. HIGH VOLTAGE AND ANALYTICAL ELECTRON MICROSCOPY
J. Bentley, E. A. Kenik, P. S. Sklad
Phone: (615)-574-5067
$500,000 01-1

Development and application of analytical transmission microscopy and HVEM to determine the microstructure and microchemistry of solids; weak-beam dark-field studies of precipitates in irradiated alloys; lattice imaging of two-phase interfaces; SAES and EELS of internally oxidized refractory metal alloys; structure of long-range ordered alloys; in situ deformation, oxidation, and hydriding studies in the 1-MeV microscope; grain boundary phases in structural ceramics; structure of metallic glasses; standardless EELS analysis.

OAK RIDGE NATIONAL LABORATORY (continued)

151. DEFORMATION AND MECHANICAL BEHAVIOR OF STRUCTURAL MATERIALS

M. H. Yoo, J. Schneibel, C. L. White, G. F. Petersen
Phone: (615)-574-5165
$625,000 01-2

Experimental and theoretical studies of effects of impurities and interfaces on deformation and fracture of Ni, Fe-Ni, Ni-Cr, Fe-Ni-Cr alloys; grain boundary cavity nucleation and growth; segregation of impurities to grain boundaries and creep cavities; dynamic recrystallization; small-angle neutron scattering studies of cavity growth during creep and fatigue in nickel and austenitic stainless steel.

152. MECHANICAL PROPERTIES OF CERAMICS

P. F. Becher, M. K. Ferber, C. J. McHargue, C. S. Yust, P. Angelini
Phone: (615)-574-5157
$500,000 01-2

Flexure strength, fracture toughness, and erosion resistance of TiB$_2$ as related to microcracking, slow crack growth and microstructure; wear studies of TiB$_2$, SiC, Al$_2$O$_3$, and transformation-toughened Al$_2$O$_3$-Zr$_2$O$_3$; slow crack growth and in situ electron microscopy studies of transformation-toughened Al$_2$O$_3$-Zr$_2$O$_3$; microhardness, indentation fracture toughness, and flexure strength of ion implanted Al$_2$O$_3$, SiC, and TiB$_2$.

153. KINETICS AND MECHANISMS OF SURFACE AND SOLID STATE REACTIONS

J. V. Cathcart, R. E. Druschel, R. A. McKee, R. E. Pawel
Phone: (615)-574-4925
$750,000 01-3

Defect interactions during diffusion and during growth of surface layers; kinetics of sulfur reactions with Fe-base alloys, definition of the electronic-ionic defect structure of FeS; diffusion in sulfur-doped oxides; stress generation and relaxation in sulfide scales; sulfur attack of ion implanted Fe-base alloys. Theoretical treatment of vacancy and interstitial diffusion in compounds having high defect concentrations.

154. METASTABLE MATERIALS

C. C. Koch, A. Das Gupta, D. S. Easton, J. A. Horton, D. M. Kroeger
Phone: (615)-574-5156
$525,000 01-3

Influence of inhomogeneous deformation on structure; stability of binary and ternary metallic glasses; critical cooling rates for glass formation; preparation techniques by arc-hammer, melt spinning, and electron-beam vapor deposition; mechanical properties of metastable materials; low temperature specific heat; small-angle x-ray and TEM studies of defect structure and phase separation in Mo-Ru-B.

OAK RIDGE NATIONAL LABORATORY (continued)

155. RADIATION EFFECTS
L. K. Mansur, R. E. Clausing, K. Farrell, M. B. Lewis, N. H. Packan, L. L. Horton, E. H. Lee
Phone: (615)-574-4797
$1,400,000 01-4

Neutron damage in pure metals, alloys, and ceramics irradiated in ORR, HFIR, and EBR-II, effect of alloying additions, impurities and microstructure on void nucleation and growth; phase stability under irradiation; damage simulation studies using multiple ion beams (heavy and dual light ions), relationship between ion and neutron damage, effect of helium and other gases on nucleation and growth of voids and interstitial loops; theoretical studies of void and loop nucleation and growth, solute-defect interactions, irradiation creep, HVEM irradiations; Al, Zr, Ni and alloys, stainless steels, ferritic alloys, ceramics.

156. FUNDAMENTAL STUDIES IN WELDING
S. A. David, J. M. Vitek
Phone: (615)-574-4804
$375,000 01-5

Control of weld microstructure through control of solidification parameters; composition, distribution, and stability of microphases; microstructure of laser-produced welds; modeling of solidification processes; austenitic steels.

157. RESEARCH IN CERAMIC PROCESSING
P. F. Becher, C. B. Finch, C. J. McHargue, P. Angelini
Phone: (615)-574-5157
$325,000 01-5

Near-surface modification of Al_2O_3, SiC, Si_3N_4, and TiB_2 by ion implantation, structure determination by Rutherford backscattering and TEM, annealing; liquid phase sintering of TiB_2; sol gel powder preparation and microstructural control in transformation-toughened Al_2O_3-ZrO_2 and Al_2O_3-HfO_2; crystal growth of β′-sialon and mullite.

158. HIGH TEMPERATURE ALLOY DESIGN
C. T. Liu, J. A. Horton, A. DasGupta
Phone: (615)-574-4459
$200,000 01-5

Ductile polycrystal alloys based on Ni_3Al; microalloying with B; macroalloying with Fe, Hf, Ce; creep, oxidation and physical properties; structure and composition of grain boundaries.

OAK RIDGE NATIONAL LABORATORY (continued)

Solid State Division - 02 -

M. K. Wilkinson - Phone (FTS) 624-6151 or 615-574-6151
F. W. Young, Jr. - Phone (FTS) 624-5501 or 615-574-5501

159. INTERATOMIC INTERACTIONS IN CONDENSED SYSTEMS
R. M. Nicklow, J. W. Cable, H. R. Child, S. Funahashi, E. Gurewitz, S. Kawarazaki, W. C. Koehler, H. A. Mook, R. M. Moon, O. A. Pringle, H. G. Smith
Phone: (615)-574-5240
$995,000 02-1

Inelastic neutron scattering studies of phonons, magnons, and single-particle excitations in condensed matter; elastic and inelastic scattering of polarized and unpolarized neutrons by magnetic materials; lattice dynamics of α-Ce, Tl, SmB_6, LaF_3, and intercalated graphite; magnetic excitations in amorphous materials, MnP, and Er; phase transitions in MnP, $PrAg_{1-x}Cu_x$, and random field systems; magnetic form factors of mixed-valence materials; structures of composition modulated systems.

160. PROPERTIES OF DEFECTS, SUPERCONDUCTORS, AND HYDRIDES
R. M. Moon, R. Arons, J. W. Cable, H. R. Child, W. C. Koehler, H. A. Mook, R. M. Nicklow, O. A. Pringle, H. G. Smith, G. D. Wignall
Phone: (615)-574-5234
$705,000 02-1

Elastic, inelastic, and small-angle scattering of neutrons by superconductors, metal hydrides, and defects in single crystals; lattice dynamics of α-U, A15 compounds, $PdTe_2$, metal alloys, and Na β''-alumina; proton diffusion in biological systems; magnetic structures in GdD_2 and reentrant superconductors; SANS from coal solutions, oil shale, surfactants, metal alloys, and polymer blends; kinetics of spinodal decomposition.

161. SUPPORT FOR NEUTRON USERS' PROGRAM (also see page 160)
H. A. Mook, J. W. Cable, H. R. Child, R. M. Moon, R. M. Nicklow, O. A. Pringle, H. G. Smith
Phone: (615)-574-5242
$260,000 02-1

ORNL neutron scattering facilities are available to outside scientists through Neutron Users' Program; recent investigations include lattice dynamics of intercalated graphite, structure of spin glasses, random field systems, metallic superlattices, proton diffusion in biological systems, and collagen periodicity in bones.

OAK RIDGE NATIONAL LABORATORY (continued)

162. PHYSICAL PROPERTIES OF SUPERCONDUCTORS
S. T. Sekula, Y. K. Chang, D. K. Christen, H. R. Kerchner, D. H. Lowndes,
J. R. Thompson
Phone: (615)-574-6271
$405,000 02-2

Investigations of flux-line-lattice arrays, flux flow, flux creep, flux-line defect interactions, and anisotropy in refractory metal alloys and compounds with A15 and B1 crystal structures; small-angle neutron scattering by flux-line lattices in equilibrium and metastable configurations, dc magnetization, ac magnetic permeability, critical-current and normal-state electrical transport; ion damage and implantation in foil and thin film superconductors; low-temperature laser quenching of superconductors.

163. PHOTOPHYSICAL PROCESSES IN SEMICONDUCTORS AND SOLAR ENERGY CONVERSION
R. F. Wood, R. B. James, G. E. Jellison, D. H. Lowndes, J. Narayan,
R. D. Westbrook, C. W. White, R. T. Young
Phone: (615)-574-5781
$820,000 02-2

Effects of point defects, defect clusters, dislocations, stacking faults, and chemical impurities on electrical and optical properties of single-crystal and polycrystalline Si; fabrication of high-efficiency Si solar cells by laser techniques; thermal and laser annealing of lattice damage in Si and GaAs; laser-induced recrystallization of amorphous layers; electrical, optical (including infrared and luminescence spectroscopy), transmission electron microscopy, x-ray scattering, surface photovoltage, secondary ion mass spectrometry, and Rutherford ion backscattering property measurements; dopant concentration profiles, deep-level transient spectroscopy, and absolute quantum efficiency measurements; fabrication of test solar cells; solar cell modeling; factors affecting degradation of solar cell conversion efficiency under single-sun and concentrator conditions; thin-film deposition on prepared substrates; chemical vapor deposition of Si on low-cost substrates; time-resolved optical measurements of laser-induced melting and recrystallization; picosecond laser spectroscopy, laser-induced photochemical deposition.

164. FUNDAMENTAL ASPECTS OF FRACTURE
S. M. Ohr, S.-J. Chang, T. S. Noggle, C. G. Park
Phone: (615)-574-5509
$405,000 02-2

Experimental and theoretical investigations to relate phenomena of continuum fracture mechanics to microscopic physical phenomena occurring at a crack tip; in situ transmission electron microscope observations of crack propagation in aluminum, copper, nickel, molybdenum, niobium, tungsten, stainless steel, magnesium oxide, and niobium oxide; crack propagation in metals containing helium bubbles; distribution of dislocations in the plastic zone ahead of crack tip in metals and ceramics; cyclic deformation; ductile-brittle transition in bcc metals; dislocation theory of J-integral; theory of plastic zone with a dislocation-free zone.

OAK RIDGE NATIONAL LABORATORY (continued)

165. SCATTERING OF SYNCHROTRON RADIATION
B. C. Larson, J. F. Barhorst, T. S. Noggle, J. Z. Tischler, C. W. White
Phone: (615)-574-5506
$130,000 02-2

Transient effects associated with pulsed-laser annealing; defect structures and defect correlations in solids; x-ray diffuse scattering; energy-resolved x-ray scattering; quasi-elastic scattering; phase transformations.

166. PHYSICAL PROPERTIES OF CERAMICS
F. A. Modine, Y. Chen, G. R. Gruzalski, T. M. Haywood, J. R. Martinelli, E. Sonder, K. L. Tsang, R. A. Weeks
Phone: (615)-574-6287
$680,000 02-2

Transition-metal carbides and nitrides and the $MgO-Al_2O_3-SiO_2$ class of refractory oxides; physical properties of materials characterized with regard to composition, defect structures, and phase segregation; studies of solid state reactions involving charge and mass transport with emphasis on materials degradation and high-temperature effects; techniques include optical and paramagnetic resonance spectroscopies, electrical properties measurements, and laser heating.

167. SOLID ELECTROLYTES AND SUPERIONIC CONDUCTIVITY
J. B. Bates, G. M. Brown, W. E. Brundage, D. Dohy, N. J. Dudney, B. C. Larson, J. C. Wang
Phone: (615)-574-6280
$385,000 02-2

Mechanisms of high ionic conductivity in the beta- and beta"-aluminas; effects of composition and crystal-growth conditions on conductivity; thermodynamics and kinetics of the hydration reactions of beta- and beta"-aluminas; effect of intercalated water on ionic conductivity; structural and dynamical properties of ionic conductors; electrical properties of beta"-alumina cermets; techniques include measurements of electrical conductivity and dielectric constant, Raman scattering, infrared absorption, neutron and x-ray diffraction, and x-ray diffuse scattering; experimental results interpreted and correlated by means of model calculations.

168. SMALL-ANGLE X-RAY SCATTERING (also see page 166)
W. C. Koehler, J. S. Lin, S. Spooner
Phone: (615)-574-5232
$130,000 02-2

Small-angle x-ray scattering of metals, alloys, polymers, and surfactants; void distributions in oil shale and irradiated metals; dynamic deformation studies of polymers; time-slicing studies of phase transformations. Facilities are available to users through National Center for Small-Angle Scattering Research (NCSASR).

OAK RIDGE NATIONAL LABORATORY (continued)

169. PREPARATION AND CHARACTERIZATION OF RESEARCH MATERIALS

L. A. Boatner, M. M. Abraham, W. E. Brundage, Y. K. Chang, L. S. Darken
Phone: (615)-574-5492

$655,000 02-2

Development of new techniques for growth of single-crystal research specimens and for preparation of advanced materials; techniques for preparation of single crystals with specified geometries; flux growth of single crystals of fast-ion conductors (β-alumina, β''-alumina); Czochralski and float-zone growth of crystals of Fe-Ni-Cr alloys (i.e., stainless steels); growth of refractory metal crystals (Ti, V, Zr, Nb, Ta, W, Ir, Re) using electron-beam float-zone technique; rf induction float-zone growth of transition-metal carbides; growth of perovskite-structure oxides ($KTaO_3$, $KTa_{1-x}Nb_xO_3$) and semiconducting oxides for photoelectrochemical cell electrodes; float-zone and tri-arc growth of crystals of A15 compounds such as V_3Si, V_3Ge, and Ti_3Pt; arc-fusion and flux growth of crystals of high-temperature materials (WC, Y_2O_3, MgO, CaO, SrO); characterization of high-quality single crystals of metals, alloys, and insulators.

170. THEORY OF CONDENSED MATTER

J. F. Cooke, J. H. Barrett, H. L. Davis, L. J. Gray, T. Kaplan, S. H. Liu, M. E. Mostoller, O. S. Oen, A. K. Rajagopal, M. Rasolt, M. T. Robinson, J. C. Wang, R. F. Wood
Phone: (615)-574-5787

$1,200,000 02-3

Theory of laser annealing, laser-induced diffusion, and nonequilibrium solidification in semiconductors; superionic conductivity and solid electrolytes; computer simulation of radiation damage and sputtering; radiation damage analysis procedures; correlation of neutron damage with ion bombardment; radiation emitted by channeled electrons and positrons; reflection of light atoms from surfaces; surface studies with backscattered ions; development of LEED theory and interpretation of LEED data; crystallography of laser-annealed semiconductors; surface vibrations and relaxation; correlation contributions to surface energy; optical potential for electron spectroscopies; theory of angular affects in photoemission and Auger emission of electrons from surface regions; electron screening; lattice dynamics of transition metals; magnetism in transition metals; Brillouin zone integration; Heisenberg spin systems; metal-hydrogen interactions; high-temperature oxides and carbides; electronic properties of amorphous systems; lattice vibrations in disordered alloys; coherent potential approximation; vibrational properties around substitutional impurities in insulators; neutron scattering from crystals and molecular-like impurities in crystals; electronic properties of rare-earth and actinide compounds; band structure calculations for metals and insulators; electronic properties of mixed-valent systems; critical phenomena and phase transitions.

OAK RIDGE NATIONAL LABORATORY (continued)

171. X-RAY DIFFRACTION AND ELECTRON MICROSCOPY
B. C. Larson, J. F. Barhorst, J. Narayan, T. S. Noggle, S. M. Ohr,
S. Pennycook, J. Z. Tischler
Phone: (615)-574-5506
$665,000 02-4

Structure of intrinsic and induced defects in solids; transmission electron microscopy; x-ray diffuse scattering; x-ray topography; defect clusters resulting from fast neutron and ion irradiations of metals; pulsed-laser annealing; defects associated with laser and thermal processing of pure and ion-implanted semiconductors; cell structure in doped semiconductors; grain boundaries in semiconductors; high-resolution atomic imaging of defects; structure of displacement cascades in silicon; solid-phase recrystallization in semiconductors; structure of high-temperature metal carbides; defects in high-temperature oxides; anisotropic elastic theory of dislocation loops; computer simulation of electron microscopy images; calculation of diffuse scattering from dislocation loops and solute precipitates; theory of interactions of electrons and X rays with defects in solids.

172. GASES IN METALS
R. R. Coltman, Jr., D. B. Poker, J. M. Williams
Phone: (615)-574-6263
$105,000 02-4

Interactions of light gas atoms with defects in metals; diffusivity of ion-implanted He in Ni, Cu, and stainless steels at low temperatures.

173. NATIONAL LOW-TEMPERATURE NEUTRON IRRADIATION FACILITY
R. R. Coltman, Jr., C. E. Klabunde
Phone: (615)-574-6263
$200,000 02-4

Design, construct, test, and operate for users a National Low-Temperature Neutron Irradiation Facility (NLTNIF) at ORNL Bulk Shielding Reactor (BSR); determine neutronics characteristics in the irradiation cryostat for use at an in-core position and with several radiation modifying devices; provide data acquisition and computer equipment for users; design and construct specialized cryogenic test equipment; provide equipment and procedures for the transfer of irradiated specimens at 4.2 K.

OAK RIDGE NATIONAL LABORATORY (continued)

174. SURFACE PHYSICS AND CATALYSIS
L. H. Jenkins, H. L. Davis, W. Erly, J. R. Noonan, G.-C. Wang,
J. F. Wendelken, C. W. White, D. M. Zehner
Phone: (615)-574-7031
$870,000 02-5

Studies of crystallographic and electronic structure of clean and adsorbate-covered metal and semiconductor surfaces with emphasis on surfaces which either reconstruct or have interplanar spacings different from those of the bulk; combined techniques of low-energy electron diffraction (LEED), positive ion crystallography of surfaces (PICS), photoelectron spectroscopy (PES) using synchrotron radiation, and computer simulations for surface crystallography studies; LEED, PES, and Auger electron spectroscopy (AES) combined with in situ laser annealing of semiconductors; lineshape analysis of Auger spectra; LEED, AES and x-ray photoelectron spectroscopy (XPS) studies of both clean and adsorbate-covered surfaces of metals and intermetallic compounds; determination of effects of intrinsic and extrinsic surface defects on surface properties using LEED; vibronic structure of adsorbates examined by high-resolution electron energy loss spectroscopy (EELS); examination of surface electronic and geometric structures with respect to solid state aspects of heterogeneous catalysis.

175. ION-BEAM ANALYSIS AND ION IMPLANTATION
B. R. Appleton, J. H. Barrett, G. M. Beardsley, R. J. Culbertson,
G. C. Farlow, O. W. Holland, E. J. Kelly, C. J. McHargue, J. Narayan,
T. S. Noggle, D. B. Poker, J. B. Roberto, O. E. Schow III, C. W. White,
J. M. Williams, S. P. Withrow
Phone: (615)-574-6283
$825,000 02-5

Positive ion crystallography of surfaces (PICS); ion-solid interactions (particulary ion channeling); pulsed-laser annealing and rapid solidification; high-speed nonequilibrium crystal growth; investigations of segregation, constitutional supercooling, solute trapping, and precipitate formation; mechanisms limiting maximum substitutional concentrations during rapid solidification; supersaturated substitutional alloys; new metastable phases and amorphous alloys fabricated by ion-beam and pulsed-laser processing; rapid thermal annealing; solid-phase epitaxial regrowth; fundamental ion damage mechanisms; applications of ion implantation doping and pulsed-laser processing to studies of corrosion/catalysis mechanisms, to reduction of friction and wear of metal surfaces, to improvements in hardness and fracture toughness of ceramics, to improvements in high-temperature materials, and to superconducting materials fabrication; ion-beam and pulsed-laser mixing in metals, semiconductors, and insulating substrates.

OAK RIDGE NATIONAL LABORATORY (continued)

176. SURFACE MODIFICATION AND CHARACTERIZATION FACILITY AND COLLABORATIVE RESEARCH CENTER (also see page 176)
B. R. Appleton, O. E. Schow III, and C. W. White
Phone: (615)-574-6283
$370,000 02-5

SMAC facility provides for alteration of materials properties in UHV by ion implantation doping, pulsed-laser processing, and ion-beam mixing at sample temperatures from 4–1300 K; in situ materials characterization by ion-beam analysis, ion channeling, electrical measurements, and surface analysis techniques; SMAC facility supports research in the Ion-Beam Analysis and Ion Implantation Program and other ORNL divisions; SMAC facility is available to scientists outside ORNL for collaborative research projects through the SMAC Collaborative Research Center.

177. RADIOACTIVE WASTE STORAGE
L. A. Boatner, M. M. Abraham, B. C. Sales
Phone: (615)-574-5492
$405,000 02-5

Research and development relating to use of synthetic analogs of monazite forms for disposal of commercial, U.S. defense, and transuranic wastes; growth of actinide-doped single crystals of monazites; determination of valence states and site symmetries of actinide and other impurities using electron paramagnetic resonance, x-ray, optical, and Mössbauer techniques; leaching of radioactive ions from orthophosphates and borosilicate glass under various conditions; use of molten urea process for production of orthophosphate powders with controlled particle sizes; compaction and microstructural characterization of hot-pressed or cold-pressed, sintered orthophosphate bodies; studies of heavy-particle-induced radiation effects in lanthanide orthophosphate compounds; investigations of mechanisms of borosilicate glass corrosion using Rutherford backscattering depth profiling, ion implantation, and surface analytical techniques.

178. RESEARCH AND DEVELOPMENT - ISOTOPE RESEARCH MATERIALS PREPARATION
H. L. Adair, W. S. Aaron, M. Petek, T. C. Quinby, D. W. Ramey
Phone: (615)-574-5901
$330,000 02-5

Research and development in preparation techniques involved with isotope-containing samples in the form of ultra-thin films (supported and self-supported), wires, rods, cast shapes, alloys, ceramics, cermets, distilled metals, inorganic and refractory compounds, matrix-dispersed materials, and liquids; techniques of preparation include vapor deposition, ion sputtering, rolling, chemical vapor deposition, liquid phase and conventional sintering, hot pressing, electrodeposition, molecular plating, zone refining, reactive and ordinary spray calcination, inorganic chemical methods; characterization of prepared research samples includes x-ray and electron diffraction, electron microscopy (TEM and SEM), microprobe studies, differential thermal analysis, thermal conductivity determinations, resonating crystal thickness monitoring, x-ray fluorescence, radiation counting (low geometry and absolute), and microweighing; phase diagram determinations for compounds and metals; all development efforts equivalent for stable and light and heavy radioactive materials.

OAK RIDGE NATIONAL LABORATORY (continued)
P. O. Box X
Oak Ridge, Tennessee 37830

Chemistry Division -03-

O. L. Keller — Phone (FTS) 624-4987 or 615-574-4987

179. CHEMICAL STRUCTURE OF ENERGY RELATED MATERIALS
W. R. Busing, B. K. Annis, G. M. Brown, A. H. Narten, D. W. Noid, W. E. Thiessen
Phone: (615)-574-4976
$820,000 03-1

Atomic and molecular arrangements in crystals and in liquids determined by neutron and x-ray diffraction studies; atom-atom pair correlation functions for liquids; small-angle neutron scattering; development of synchrotron radiation facilities. Computational methods for dynamic correction of neutron scattering intensities; improvement of statistical mechanics for understanding molecular fluids and for extrapolating their physical properties; use of intermolecular and intramolecular potentials to interpret the conformation of molecules in crystals; calculation of physical properties of crystals. Materials studied include superionic conductors for use in high-temperature batteries and fuel cells, alloys with unusual thermal properties, hydrocarbon fuels, compounds which are potential catalysts for hydrogenation and hydrogen production, water and aqueous lanthanide and actinide solutions, and silicate minerals of geochemical interest.

180. HIGH TEMPERATURE CHEMISTRY AND THERMODYNAMICS OF STRUCTURAL MATERIALS
C. E. Bamberger, J. Brynestad, G. M. Begun
Phone: (615)-574-4944
$640,000 03-2

Synthesis of high-purity structural ceramic compounds by novel reactions; emphasize exothermic homogeneous (gas-phase) and heterogeneous (gas-solid) reactions that yield extremely fine powders; reactions of titanium and titanium chlorides with gaseous BCl_3 to yield TiB_2 powder with particle size of 100 nm or less; reactions of BCl_3 with commercial TiB_2 to remove oxide contamination; reaction of $TiCl_2$ or $TiCl_3$ with N_2 or NH_3 to yield TiN; reaction thermodynamics and mechanisms; compaction and sintering studies.

OAK RIDGE NATIONAL LABORATORY (continued)

Chemistry Division -03-

181. LOCALIZED CORROSION AND STRESS CRACKING PHENOMENA RELATED TO ENERGY TECHNOLOGIES
F. A. Posey, A. L. Bacarella, H. R. Bronstein, G. M. Brown,
E. J. Kelly, C. E. Vallet
Phone: (615)-574-5022
$700,000 03-3

Use of ion implantation/Rutherford backscattering techniques with electrochemical methods in basic studies of mechanisms of aqueous corrosion reactions occurring in localized attack of metals (titanium, vanadium, molybdenum, etc.); investigation of electrochemical and corrosion properties of precisely-defined surface alloys (Ti-Pt, Ti-Mo, Ti-V, etc.); effects of soluble redox systems [Ti(IV)/Ti(III), V(IV)/V(III)/V(II), etc.] on localized corrosion of titanium; hydrolysis and speciation effects on interfacial reaction kinetics in concentrated aqueous electrolytes encountered in localized corrosion; application of photoacoustic spectroscopy coupled with electrochemical measurements to in-situ corrosion studies (film formation, surface concentrations and identity of reaction intermediates, etc.).

OAK RIDGE NATIONAL LABORATORY (continued)
P. O. Box X
Oak Ridge, Tennessee 37830

Chemical Technology Division -03-

R. G. Wymer - Phone (FTS) 624-6275 or 615-574-6275

182. THERMODYNAMICS AND SENSITIVITY ANALYSES INVOLVING ENERGY RELATED MATERIALS
T. B. Lindemer, T. M. Besmann, C. A. Culpepper
Phone: (615)-574-6850
$262,000 03-2

Determination and modeling of phase equilibria and other thermochemical data critical to relevant energy-producing systems. Studies involve relevant subsystems in the system of elements U, Pu, Th, C, O, and specific fission products, particularly lanthanides. Second- and third-law determinations of the entropies and enthalpies of formation of relevant compounds. Modeling of nonstoichiometric actinide oxide, fluorite solid solutions. Development of generalized mathematical analyses to permit identification of those phases for which thermodynamic data must be known most precisely.

183. CHEMICAL ENGINEERING RESEARCH
D. F. Williams, C. H. Byers
Phone: (615)-574-4653
$262,000 03-2

Fundamental laser scattering measurements and theoretical framework for material transport and thermodynamic properties of liquid mixtures at high temperatures and pressures, often in the critical region. Methods development (including optical measurements, dispersion stabilization, and mathematical analysis) for properties measurement of organic mixtures such as those important in critical extraction and those found in coal conversion streams. Viscosities, diffusivities, and interfacial properties at high pressures and temperatures. Associated thermodynamic properties measurement, correlation and development of predictive relationships. High pressure vapor-liquid equilibrium measurements.

PACIFIC NORTHWEST LABORATORY
P. O. Box 999
Richland, Washington 99352

Materials Science Division -01-

S. D. Dahlgren - Phone (FTS) 444-0120 or 509-376-0120

184. HIGH TEMPERATURE CORROSION AND ELECTROCHEMICAL INTERACTIONS IN CERAMICS
J. L. Bates and D. D. Marchant
Phone: (509) 375-2579
$105,000 01-1

Mechanisms and kinetics of high temperature reactions of refractory metal oxides with molten silicates and gases in coal-derived environments; dissolution of oxides in liquid silicates by molecular diffusion and natural/forced convection; mass transport and diffusion studies near reaction interfaces as determined from elemental distribution using optical microscopy, SEM, quantitative electron microprobe, STEM, surface and near surface analyses; reaction studies of $MgAl_2O_4$, MgO or Al_2O_3 with liquid CaO-Al_2O_3-SiO_2 containing iron and magnesium. Electrochemical interactions of oxides in molten electrolytes, effect of structure on electrochemical decompositions, and evaluation of reactions between oxides, molten salts and silicates; refractory oxides include ionic and electronic conductors; effect of structure on electrochemical decompositions, and evaluation of reactions between oxides and molten salts and silicates.

185. SPUTTER DEPOSITED AMORPHOUS SEMICONDUCTORS
P. M. Martin and W. T. Pawlewicz
Phone: (509) 375-2076
$90,000 01-1

Study the effects of composition and microstructure on the electrical and optical properties and residual stress in sputtered thin film amorphous semiconductors. Develop models of reaction kinetics and film-plasma interactions occurring during the reactive sputtering process. Explore relationships between local bonding and configurations, stoichiometry and microstructure. The properties of Si_3N_4:H are currently being investigated. Measurements are being made on residual stress, bonding, phase composition and stoichiometry. Electrical property determinations include temperature dependent resistivity, Hall effect, C-V and I-V characteristics. Optical properties under investigation are refractive index, infrared vibrational absorptions and the fundamental interband absorption edge. Measurement techniques include optical and infrared spectroscopy, Raman spectroscopy, in, electrical transport measurements, C-V and I-V analysis, XPS, x-ray diffraction and x-ray fluorescence.

PACIFIC NORTHWEST LABORATORY (continued)

186. EFFECT OF COAL MICROSTRUCTURE ON PROPERTIES

J. M. Lytle and L. R. Bunnell
Phone: (509) 375-2254

$90,000 01-1

Quantitative characterization of coal properties including mechanical, fracture, microstructural, and compositional; determination of the modes and mechanisms of fracture during coal comminution and the interrelationships between coal properties and fracture modes and mechanisms; determination of fracture properties of coal particles including load-displacement relationships, energy to fracture and the effect of heat, liquid, and/or sonic treatments on fracture properties; determination of the effects of both 1) energy to fracture in slow compression tests and 2) milling time in ball milling tests on the shapes of particles produced; determination of porosity, surface area, and pore size distribution as a function of ball milling time.

187. FUNDAMENTAL STUDIES OF STRESS CORROSION AND CORROSION FATIGUE MECHANISMS

R. H. Jones, M. T. Thomas, S. M. Bruemmer, D. R. Baer and M. J. Danielson
Phone: (509) 376-4276

$335,000 01-2

Investigation of the mechanisms controlling intergranular and transgranular stress corrosion and corrosion fatigue cracking of iron, iron-chromium-nickel and nickel-based alloys in gaseous and aqueous environments. Computer modeling and experimental measurements of surface and grain boundary segregation of S, P, Sb, C, N, and O in Fe and Ni as a function of time, temperature, and bulk concentration. Relationships between grain boundary chemistry, electrochemical potential, fracture mode, ductility, crack growth rate and fracture thresholds of Fe and Ni in aqueous solutions are being studied. Modeling of the electrochemical conditions at the tip of a growing crack and evaluation of the electrochemical behavior of sulfur and phosphorus in the grain boundaries of nickel. Effect of plastic strain and various gaseous environments (H_2S, Cl^-, NH_3) on the quantity and distribution of surface adsorbates is being studied by Auger Electron Spectroscopy using an in-situ straining stage.

188. OXIDATION AND CORROSION RESISTANT FINE-GRAINED MATERIALS

J. T. Prater and D. R. Baer
Phone: (509) 375-6905

$120,000 01-3

Investigate the mechanisms controlling the high-temperature corrosion of sputter-deposited fine-grained materials. Oxidation and sulfidation studies are being performed on stainless steel in $CO-CO_2$ and $CO-CO_2-H_2S$ gaseous environments at 800 to 1000°C, and hot corrosion studies are being conducted on MCrAlY covered with Na_2SO_4 in an SO_2-O_2 atmosphere at 650 to 800°C. AEM, micro-focus x-ray diffraction and mechanical tests are being used to determine the effect alloy grain size, alloying additions, and gaseous environment have on scale microstructure, scale adherence and scale cracking behavior. AES, XPS, and nuclear microprobe measurements are employed to determine the diffusion and chemical state of elements at the alloy surface during the corrosion process.

PACIFIC NORTHWEST LABORATORY (continued)

189. LEACHING OF GLASS AND CERAMICS
G. L. McVay, L. R. Pederson and D. S. Goldman
Phone: (509) 375-3672
$110,000 01-3

Mechanistic investigations of the reactions of silicate glasses and crystalline ceramics with aqueous solutions. Studies of the role of surface potential, structure, solubility, sorption, thermodynamic properties, reaction layer buildup, and chemical properties of solutions on leachability. Analytical techniques include zeta potential, radioactive and nonradioactive tracers, Rutherford backscattering spectrometry, nuclear reaction analysis, Raman scattering spectrometry, X-ray photoelectron spectroscopy, secondary ion mass spectrometry, and Fourier predictive model for glass/water interactions.

190. RADIATION EFFECTS IN METALS AND CERAMICS
E. P. Simonen, J. L. Brimhall, G. J. Exarhos, E. R. Bradley,
L. A. Charlot, C. H. Henager, Jr., H. E. Kissinger, R. Wang,
and W. J. Weber
Phone: FTS 444-3124
$630,000 01-4

Evaluation of radiation damage mechanisms in metals and non-metals; irradiation of metals using heavy-ion and neutron bombardment; analyses using analytical electron microscopy, positron annihilation, rate theory microstructural modeling; in-situ irradiation creep testing; effects of irradiation and substructure on creep, recovery, recrystallization, defect microstructures and hardening; pulsed irradiation effects on microstructures; effects of primary damage on amorphous and crystalline phase stability and corrosion resistance; studies of nickel, molybdenum, ferritics, amorphous metals, and ordered intermetallic compounds. Dose and dose rate dependence of damage ingrowth in non-metallic solids resulting from internal alpha decay events, external ion bombardment, or gamma irradiation. Characterization of localized defect states in crystals and glasses by vibrational Raman spectroscopy and optical absorption techniques. Kinetic studies of damage ingrowth and annealing phenomena using x-ray diffraction, electron microscopy, and bulk swelling determinations. Model development for the damage state in insulators with an emphasis on radiation induced structural changes in glassy silicates and phosphates.

191. SPUTTERING PARAMETER INFLUENCES ON MATERIAL STRUCTURE AND BEHAVIOR
R. W. Knoll, E. D. McClanahan, and W. T. Pawlewicz
Phone: (509) 375-6902
$220,000 01-5

Synthesis of metallic alloys, ceramic, and dielectric materials by sputter deposition and reactive sputtering. Characterization of microstructure, structure and properties are being made that include phase transformations using x-ray diffraction, TEM, SEM, AES, thermal analysis, as well as electrical and optical measurements. Emphasis is on unique nonequilibrium or metastable phases and composites. Definition of the deposition process and relation between process parameters and material characteristics are being explored. Material systems include rare earth/transition metal alloys, refractory metal alloys, binary and ternary oxides.

PACIFIC NORTHWEST LABORATORY (continued)

192. SPUTTER-DEPOSITED COATINGS FOR OPTICAL APPLICATIONS

W. T. Pawlewicz, P. M. Martin, and D. D. Hays
Phone: (509) 375-2074
$135,000 02-2

Study of the optical properties of dielectric materials in thin-film form. Oxides, nitrides and elemental semiconductors are currently under investigation. Work includes measurement, modeling and understanding of relationships between optical properties and materials properties. Materials properties are controlled through understanding of the reactive sputtering process. Optical properties of interest are: spectral dependence of the complex refractive index; fundamental interband and lattice vibrational absorption edges; scattering; optical homogeneity, uniformity and isotropy. Related materials properties are: structure, microstructure, bonding in amorphous materials, stoichiometry, composition, purity and surface topography. Measurement techniques include transmission and reflection spectrophotometry, total integrated scattering, x-ray diffraction, Raman spectroscopy, STEM, x-ray fluorescent analysis, Nomarski microscopy, and interferometry.

193. OPTICAL AND LASER MATERIALS STUDY

J. W. Griffin and J. S. Hartman
Phone: (509) 375-2081
$125,000 02-2

Research to establish correlations between physical properties and optical losses (scattering and absorption) in optical thin films (coatings). Identify loss mechanisms; develop loss models for prediction of coating performance; provide suggestions for minimization of absorptive and scattering losses through variation of materials components, coating geometry, surface treatment and/or coating synthesis procedures. Optical diagnostic techniques include total integrated scatter (TIS), angular scattering distribution, precision spectrophotometry (reflectance and transmission), photoacoustic spectroscopy (PAS), and ellipsometry. Materials systems include single and multilayer coatings of TiO_2, ZrO_2, Ta_2O_5, Nb_2O_5, SiO_2, and Si_3N_4 on dielectric substrates.

SANDIA NATIONAL LABORATORIES
P. O. BOX 5800
Albuquerque, New Mexico 87185

F. L. Vook - Phone: (FTS) 844-9304 or (505) 844-9304

194. STRESS CORROSION CRACKING AND ELECTROCHEMISTRY OF TRANSIENT CORROSION PROCESSES
W. H. Smyrl, R. J. Salzbrenner
Phone: (505) 844-6638 or FTS 844-6638
$140,000 01-2

Studies of crack propagation behavior of austenitic and ferritic stainless steels in molten NaCl-$AlCl_3$ environments. Importance of electrochemical reactions in cracking illustrated: Cl^- induced cracking rates shown to be directly proportional to rate of electrodissolution. Digital Faradaic Analysis used to study electrodissolution of Cr in molten NaCl-$AlCl_3$ and corrosion of Cu in aqueous solutions. Depletion of Cr observed (Auger analysis) to shallow depths under both transient and steady state conditions.

195. ION IMPLANTATION AND DEFECTS IN MATERIALS
P. S. Peercy, S. T. Picraux, S. M. Myers, K. L. Brower, B. L. Doyle, H. J. Stein, D. M. Follstaedt, J. A. Knapp
Phone (505) 844-4309 or FTS 844-4309
$720,000 01-3

Ion implantation and ion-beam mixing are used in conjunction with laser and electron-beam annealing to form metastable and equilibrium states within the near-surface regions of metals, semiconductors, and insulators. Microscopic characterization of modified layers is performed by ion-beam depth-profiling, ion channeling, TEM, EPR, and optical absorption. The kinetics of transient laser/electron-beam annealing are examined by calorimetry, time-resolved reflectivity and transient conductance. In equilibrium intermetallic systems, diffusion rates, phase diagrams, and solute-trapping mechanisms are determined. New metastable crystalline and amorphous alloys are produced both by ion implantation and by transient annealing; stability bounds and microstructures are determined, and resulting improvements in mechanical and corrosion properties are measured. Methods based on ion implantation and ion beam analysis are also used to characterize the behavior of hydrogen in metals, including diffusivity, solubility, surface-barrier effects, and trapping by defects, solutes, precipitates and gas bubbles. In semiconductors, the fundamental properties of defects and impurities are determined by EPR and optical absorption following their controlled introduction by ion implantation. Laser and electron-beam annealing of silicon are investigated for the removal of implantation-doping damage, for the production of single-crystal silicon on insulators, and to elucidate fundamental aspects of rapid solidification. Refractory amorphous alloys are under study for diffusion barriers or metallization of semiconductors for elevated temperature applications.

SANDIA NATIONAL LABORATORIES (continued)

196. **EROSION, WEAR AND STRESS CORROSION IN CERAMICS**
T. A. Michalske, M. L. Knotek, G. A. Fisk, R. E. Cuthrell
Phone: (505) 846-3551 or FTS 846-3551
$260,000 01-5

Crack growth and fatigue properties of glasses, oxides and brittle materials; emphasis on effects of environment on crack growth and strength; chemical models for environment/strained solid interactions used to interpret fatigue effects; environments include H_2O, H_2, O_2, CH_3OH and NH_3; fatigue response measured in vacuum and other high purity environments; crack growth studies utilize direct measurement on fracture mechanics specimens; Electron Stimulated Desorption (ESD) of in situ fracture surfaces to determine chemical compounds resulting from stress corrosion fracture; tunable IR laser used to excite specific molecular adsorbate vibrations during crack growth model systems (structures exhibiting high configurational strain) used to study strain-enhanced chemistry; FTIR studies of adsorbate reactions used to explore relationship between strain enhanced chemistry and stress corrosion fracture.

197. **SEMICONDUCTORS FOR USE AT HIGH TEMPERATURES AND STRAINED-LAYER SUPERLATTICES**
R. M. Biefeld, L. R. Dawson, I. J. Fritz, P. L. Gourley, D. R. Myers, G. C. Osbourn
Phone: (505) 844-6653 or FTS 844-6653
$300,000 01-5

Program deals with materials research in two inter-related areas of compound semiconductors: (i) semiconductors for use at high temperatures, and (ii) strained-layer superlattices. Work has a comprehensive fundamental scope and is closely integrated with modern materials growth techniques and coordinated with device physics programs to give this research technological impact. First area is motivated by a strong need for wide bandgap (Eg >1.4 eV) semiconductors for electronic devices which can operate in high temperature environments (to 500 C) such as in nuclear reactors, jet engine controls, photovoltaic concentrators, and down-hole logging in gas, oil, and geothermal wells. Second area deals with the fundamental electronic properties of the new area of strained-layer superlattices (SLS's) which is being pioneered at Sandia. SLS's represent a new class of semiconductor materials with unique and tailorable electronic and structural properties; expected to find a broad range of device applications.

SANDIA NATIONAL LABORATORIES (continued)

198. SURFACE PHYSICS RESEARCH
M. L. Knotek, D. R. Jennison, J. E. Houston, R. R. Rye, J. A. Panitz, G. L. Kellogg
Phone: (505) 844-6653 or FTS 844-6653
$310,000 02-2

Broad range of experimental and theoretical studies aimed at understanding the interaction of atoms and molecules with solid surfaces; unique local aspects of Auger Electron Spectroscopy exploited to study the variation of electronic properties during such interactions, local chemical environment of surface and adsorbed species obtained using gas-phase molecules as "absolute" standards along with theoretical analyses of the spectroscopic results; Auger applied to understand catalysis, explosive sensitivity and Si/H surface interactions. Imaging and mass spectroscopic abilities of the field-ion and field-desorption techniques developed to study the morphology of biological and other molecules. Pulsed Laser Atom Probe applied to studies of adsorption and reaction intermediate states of molecules interacting with the various planes of well defined transition metal surfaces; technique also used to observe directly adatom-adatom and adatom-defect interactions on metals.

199. ELECTRON AND PHOTON-STIMULATED DESORPTION
M. L. Knotek, G. M. Loubriel, D. R. Jennison, R. H. Stulen
Phone: (505) 844-6653 or FTS 844-6653
$275,000 02-2

Studies of metal, metal oxide, semiconductor and alkali halide surfaces as well as their interactions with H_2O, H_2, O_2 and other adsorbates using Electron- and Photon-Stimulated desorption techniques (ESD and PSD) Investigations exploit the discovery that desorption occurs by Auger decay of radiation induced core holes. Extraction of site specific, adsorbate specific electronic and structural information from both the local empty density of states (XANES) and extended x-ray absorption fine structures (EXAFS); ESD/PSD uniquely surface sensitive and sample only the uppermost layer of surface atoms. The high sensitivity to hydrogen exploited in studies of its role in catalysis, corrosion and semiconductor technology. Angle resolved photoemission and XPS using synchrotron radiation used to correlate desorption producing excitations with ground state electronic structure and many electron excitation phenomena; partial and total photoelectron yield studies to compare PSD sites to bulk sites; coincidence Auger electron/ desorbed ion measurements to determine desorption-inducing Auger final states.

SANDIA NATIONAL LABORATORIES (continued)

200. STABILITY AND CHARGE-TRANSFER PROPERTIES OF THE SOLID-LIQUID INTERFACE
M. A. Butler, D. S. Ginley
Phone: (505) 844-8863 or FTS 844-8863
$85,000 02-2

The basic charge transfer mechanisms involved in photocatalytic and photo synthetic reactions at semiconductor-electrolyte interfaces are being investigated with special attention directed at understanding the stability of these interfaces. Photoresponse measurements are used to study surface modified by ion implantation, chemisorption, or by overcoating with corrosion resistant materials. A laser scanning system has been constructed which makes photoelectrochemical measurements on semiconducting films less than 50 Å thick with a spatial resolution approaching one micron. The development of photoelectrochemical techniques for probing the solid-liquid interface will impact not only the photoelectrochemical area but should provide valuable information in the areas of catalysis, batteries and corrosion.

201. CHEMICAL VAPOR DEPOSITION RESEARCH
A. W. Johnson, W. G. Breiland, P. Ho, M. E. Coltrin
Phone: (505)-844-8782 or FTS 844-8782
$230,000 02-2

Studies of important vapor-phase reactions and nucleation processes during CVD deposition under conditions used to fabricate photovoltaic cells, corrosion-resistant coatings, and semiconductor devices. Measurements of major and minor species densities, gas temperatures, fluid flows, and gas-phase particulate distributions using laser Raman and Mie scattering and laser induced fluorescence. Test of our predictive model, which includes chemical kinetics and fluid dynamics. Study and development of laser CVD, laser photochemical deposition, laser-based physical deposition, and laser-based fabrication of small-dimension structures. Application of our laser-based measurement capabilities to the study of vapor phase reactions of these laser processing techniques and application of surface measurement techniques to study the product materials.

SANDIA NATIONAL LABORATORIES
Livermore, California 94550

Materials Science Division - 01 -

Walter Bauer - Phone (FTS) 532-2994 or (415) 422-2994

202. GASES IN METALS
W. D. Wilson, G. J. Thomas, M. S. Daw
Phone: (FTS) 532-2264 or (415) 422-2264
$230,000 01-1

This investigation of the behavior of hydrogen and helium in metals involves joint theoretical and experimental research. The experimental program involves a variety of techniques, including electron microscopy, mechanical property measurements, and small angle neutron scattering, applied to tritiated metals and also metals implanted with helium below the damage threshold. These experiments are verifying the prediction of spontaneous lattice damage by helium which were made from fundamental calculations and how this damage influences mechanical behavior. The same theory is presently being focused on helium-dislocation interactions. A new method (Embedded Atom Method) has been developed here to calculate the cohesive energy of metals and alloys with chemically active impurities. This new method is being used to investigate the atomistic processes of fracture and the effects of hydrogen. Calculations of the trapping of hydrogen by impurities and alloying additions are also being performed.

203. MECHANISMS OF HYDROGEN EMBRITTLEMENT--EFFECTS OF GASEOUS VERSUS ELECTROCHEMICAL CHARGING
S. L. Robinson, N. R. Moody
Phone: (FTS) 532-2209 or (415) 422-2209
$110,000 01-2

A program to determine the efficacy of electrochemical charging with hydrogen to simulate gaseous environments by comparing electrochemically charged and gas charged FCC and BCC alloys. Quantify the hydrogen fugacity generated by electrochemical charging, characterize interactions of electrochemical charged hydrogen with microstructural features, determine microstructural damage resulting from charging, measure effective diffusivity for electrochemical charging.

204. PROTECTIVE BARRIERS AND COATINGS FOR COMBUSTION-RELATED MATERIALS (also see page 178)
R. E. Palmer, J. C. Hamilton, A. S. Nagelberg
Phone: (FTS) 532-3126 or (415) 422-3126
$360,000 01-1

This is a program to study corrosion/erosion mechanisms in high-temperature combustion environments, utilizing optical methods to observe the attack processes. Mechanisms of hot corrosion of ceramic turbine blade coatings by molten salt deposits are being studied in both a carefully controlled laboratory furnace and an Atmospheric Combustor Exhaust Simulator, which provides a realistic hot, particle-laden flow stream. Both facilities are instrumented for in situ Raman analysis. Corrosion by mixed gas-phase oxidants will receive increasing emphasis. In situ observations are supplemented by appropriate post-exposure analysis.

SANDIA NATIONAL LABORATORIES (continued)

205. DIAGNOSTICS FOR COMBUSTION-RELATED MATERIALS RESEARCH
R. E. Palmer, R. J. Anderson, J. C. Hamilton
Phone: (FTS) 532-3126 or (415) 422-3126
$210,000 02-5

This is a program to develop laser-based diagnostic techniques for studying corrosive/erosive processes in situ and nonintrusively at high temperature. New techniques are demonstrated on an Atmospheric Combustor Exhaust Simulator, a facility available to outside users for simulating realistic combustor exhaust environments. Techniques being developed emphasize Raman scattering and other optical techniques that can monitor surface processes and oxide layers, as well as the surrounding gaseous environment, during exposure. Complementary post-exposure techniques supplement these real-time optical diagnostics.

SOLAR ENERGY RESEARCH INSTITUTE
1617 Cole Boulevard
Golden, Colorado 80401

Solar Thermal and Materials Research Division - Materials Research Branch - 01-

G.E. Gross - Phone (FTS) 327-1228 or 303-231-1228
S.R. Bull - Phone (FTS) 327-7723 or 303-231-7723

206. SOLAR MATERIALS RESEARCH
A.W. Czanderna, P. Schissel, J.D. Webb, J.R. Pitts, T.M. Thomas
Phone: (303) 231-1240
$310,000 01-1

Degradation mechanisms and bonding at interfaces between solar materials; studies of the glass/silver, silica/silver, silver/silicon, and silver/polymer systems; silver deposition by evaporation, sputtering, and electroless deposition; polycrystalline silver films characterized for reflectance, topography, structure, and elemental composition; stability of polymer/silver interfaces, with emphasis on polycarbonate and polymethymethalcrylate; degradation in simulated solar environments; UV radiation, environmental oxidizing gases, and atmospheric pressures; interfacial catalytic and corrosion effects; diffusion, SEM, EDX, XPS, SIMS, ISS, SAM, and FT-IR, reflection absorption spectroscopy.

Solar Electric Conversion Research Division - Solid State Research Branch - 02-

S. Deb - Phone (FTS) 327-1105 or 303-231-1105
S.R. Bull - Phone (FTS) 327-7723 or 303-231-7723

207. SEMICONDUCTOR THEORY
A. Zunger
Phone: (303) 231-1172
$60,000 02-3

(1) Study of the electronic properties, structural anomalies and the interrelations between the two for ternary chalcopyrite (ABX_2, where A=Cu, B=Al, Ga, In, X=S, Se) and ternary Pnictides (ABX_2, where A=Zn, Cd, B=Si, Ge, Sn, X=P, As, Sb) semiconductors. Theoretical technique: the Mixed Basis Potential Variation band structure method. (2) Electronic structure of transition atom impurities in binary semiconductors (Si, GaP). Theoretical technique: the Quasi Band Crystal Field Green's function method. (3) Theory of optical bowing in alloys of binary semiconductors (GaP-InP). (4) Applicability of the local density functional formalism and extentions to it (the self interaction correction) for studying localized states.

SECTION B

Contract Research

(Primarily Universities)

The information on pages 75-150 was prepared by the DOE project monitor in the Division of Materials Sciences. There is considerable (about 10%) turnover in the Contract Research program and some of the projects will not be continued beyond the current contract period.

ARIZONA STATE UNIVERSITY

301. IMAGING OF SURFACES AND DEFECTS OF CRYSTALS

J. M. Cowley - Dept. of Physics
Phone: (602)-965-6459

$ 97,350 02-2

Techniques of microdiffraction, imaging of surfaces using reflected diffracted electrons and electron energy loss spectroscopy applied to study of near-amorphous thin films of oxides and other corrosion products on metal surfaces and to investigations of surface reactions of various ceramic oxides. Allied development and exploration of new and improved electron-optical techniques for study of surface structures and reactions and the influence of crystal defects.

302. TRANSPORT IN SOLID ELECTROLYTES CONTAINING A DISPERSED SECOND PHASE

J. B. Wagner, Jr. - Center for Solid State Science
Phone (602)-965-6959, 4544

$ 84,917 01-3

Characterization of contribution of number and mobility of ionic charge carriers and of space charge layers to conductivity increase mechanisms in a AgI or CuCl matrix containing a second phase such as silica, MgO, flyash, etc. Role of aliovalent doping of the matrix phase. Behavioral effects due to moisture and to added dielectrics such as alcohols or hydrocarbons. SEM, variable frequency ac conductivity, and dc polarization analysis.

UNIVERSITY OF ARIZONA

303. ARTIFICIALLY LAYERED SUPERCONDUCTORS

C. M. Falco - Dept. of Physics
Phone: (602)-626-1866

$ 72,175 (7½ months) 02-2

An investigation of the structure of artificial metallic multilayer systems, their electronic and superconducting properties including their weak link characteristics. A major objective is to produce superlattices with higher perfection than has been yet achieved and to understand what are the important preparation parameters. The initial stage will be to fabricate layered materials with a three-gun magnetron sputtering system and use x-ray diffraction, resistance, Rutherford backscattering, TEM and other techniques such as electron tunneling and the superconducting properties to characterize the samples. A latter stage of the program will emphasize the superconducting properties of the superlattice systems and to develop weak links and microbridges with desireable properties such as an increased range of operating conditions.

BATTELLE COLUMBUS LABORATORIES

304. FAILURE OF CERAMICS FROM MULTIAXIAL STRESSES

A. R. Rosenfield, D. K. Shetty, S. G. Sampath, W. H. Duckworth
Phone: (614)-424-4353

$114,000 (9 months) 01-5

Response of ceramic materials to multiaxial stress states. Consideration of: (a) surface condition, (b) test geometry, and (c) environment. Control of each of the above variables so individual effects can be studied, specimen preparation to insure that the flaw population is isotropic and material directionality is eliminated. Relationship of stress-state effects to stress-intensity factor, effects of tensile and shear stresses parallel to an artificial crack and effects of stress ratios on strength in ceramic specimens containing natural flaws to evaluate statistical (Weibull) descriptions of strength. Material characterization, fractography, three dimensional linear elastic finite element analysis of test-specimen geometries and for stress-intensity factors. High-temperature biaxial tension tests of ceramic specimens containing controlled artificial flaws. Materials of interest: Al_2O_3, SiC, Si_3N_4 and glass-ceramics.

BOEING AEROSPACE COMPANY

305. X-RAY SPECTROSCOPIC INVESTIGATION OF METAMICTIZATION AND ANNEALING IN CRYSTALLINE PHOSPHATES, SILICATES, AND COMPLEX Ti-Nb-Ta OXIDES

R. B. Greegor
Phone: (206)-655-0514
F. W. Lytle
Phone: (206)-655-5574

$ 74,961 01-1

Detailed examination of the near neighbor site geometries of metal atoms in metamict minerals (e.g., A (U,Th) and B (Ti, Nb, Ta) site cations) as determined by extended X-ray absorption fine structure (EXAFS) and X-ray absorption near edge structure (XANES) spectroscopy using the SSRL. Study of radiation damage annealing and leaching mechanisms of metamict minerals. Determination of the structure of the metamict state. Assessment of long term stability of crystalline, titanate, phosphate and silicate radioactive wasteforms (e.g., SYNROC, Sandia Titanate) which would be subject to the same processes of radiation damage and geochemical alteration in applications as a primary host for radioactive wastes.

BOSTON UNIVERSITY

306. INFRARED ABSORPTION SPECTRUM OF FREE CARRIERS IN POLAR SEMICONDUCTORS: OPTICAL ABSORPTION AND ELECTRON TRANSPORT AT HIGH FIELDS IN BULK AND LAYERED COMPOUNDS

B. Jensen - Dept. of Physics
Phone: (617)-353-2610

$ 92,640 02-3

Theoretical calculations directed at the understanding of the frequency and carrier dependence of the optical absorption coefficient and effective electron scattering time from the far to near infrared frequencies for the polar semiconductors: GaAs, InP, InAs, CdTe and ZnSe; development of a quantum theory of free carrier absorption in the presence of large magnetic or electric fields.

BOSTON UNIVERSITY (continued)

307. THEORETICAL STUDIES OF THE STATICS AND DYNAMICS OF INTERCALATION

G. Kirczenow - Dept. of Physics
Phone: (617)-353-2609

$ 69,432 02-3

Effects of charge transfer, interlayer cohesion, and in-plane and elastic interactions on the equilibrium properties and growth kinetics of the phases (or stages) of graphite intercalation compounds. Research motivated both by specific interest in quantitative comparisons of theory with experiment and by more general interest in basic physics of these materials as metastable solid state systems.

BRANDEIS UNIVERSITY

308. TWO-DIMENSIONAL COLLOIDAL SYSTEMS

R. B. Meyer - Dept. of Physics
Phone: (617)-647-2231

$ 44,200 02-2

Experimental study of two-dimensional structures formed by interfacial and thin-layer colloids, especially with regard to two-dimensional melting. These colloidal systems exhibit truly two-dimensional behavior, free of periodic substrate interactions. The particle scale (0.1 to 10μm) permits both exploration of reciprocal space by coherent light scattering and direct real space observations by optical microscopy.

BROWN UNIVERSITY

309. A COMBINED MACROSCOPIC AND MICROSCOPIC APPROACH TO THE FRACTURE OF METALS

R. J. Asaro - Div. of Engineering
Phone: (401)-863-1456
J. Gurland - Div. of Engineering
Phone: (401)-863-2628
A. Needleman - Div. of Engineering
Phone: (401)-863-2863

$201,000 01-2

Theoretical and experimental approach to fracture behavior in metals, principally steels; near tip stress and strain fields for a moving crack in elastic - ideally plastic material under small scale yielding conditions; effect of yield surface vertices on crack tip fields; effect of carbide and martensite phase distribution on the fracture toughness of duel phase and high strength martensitic steels; cavitation as a function of plastic strain, particle size, stress triaxiality; creep cavity growth in deformation vs diffusion controlled regimes under multiaxial loading; validity of singularity describing crack tip strain fields during load transients.

310. STRAIN RATE EFFECTS IN THE DEFORMATION OF SOLIDS BY MEANS OF STRESS PULSE AND ULTRASONIC METHODS

C. Elbaum - Div. of Applied Mathematics
Phone: (401)-863-2186
A. Hikata - Div. of Applied Mathematics
Phone: (401)-863-2187

$ 85,000 01-2

Measurement of deformation of metals at intermediate strain rates (10^{-1} -10^{3} sec^{-1}), using the Hopkinson bar method for generating stress wave and ultrasonic methods to monitor the materials response; relationships between stress, mobile dislocation density, average velocity, and strain rate under single as well as multiple slip conditions; dislocation interaction with point defects; metals studied - Al, Fe, Nb, Ti, Zn.

311. TIME RESOLVED FAR INFRARED SPECTROSCOPY OF EXCITONS

A. V. Nurmikko - Div. of Engineering
Phone: (401)-863-2869

$ 75,782 02-2

High resolution time-resolved spectroscopy of excitons in semiconductors at infrared and far infrared wavelengths by tunable pulsed laser excitation on a subnanosecond time scale. GaP, ZnTe and other III-V and II-VI semiconductors.

CALIFORNIA INSTITUTE OF TECHNOLOGY

312. MELTING IN ADSORBED FILMS

D. Goodstein - Div. of Physics, Mathematics and Astronomy
Phone: (213)-356-4315

$ 80,000 02-2

Study on melting of solid phases in adsorbed films and relationship of two-dimensional melting to three-dimensional melting. Pulsed NMR and thermodynamic measurements for methane on graphite substrates. Analysis of experimental data for physisorbed films, including the quantum systems ^{4}He and ^{3}He on graphite, in relation to current theory.

313. STUDIES OF ALLOY STRUCTURE AND PROPERTIES

W. L. Johnson - Div. of Engineering and Applied Science
Phone: (213)-356-4433

$230,000 01-1

Synthesis, structure and properties of amorphous alloys; electronic structure and superconductivity; flux pinning by crystalline precipitates; low temperature calorimetry; magnetic impurities and ordering in superconductors; local chemical and physical structure using AXD, EXAFS, X-ray Raman scattering and Mössbauer techniques; measurements of creep, ductility, yield strength and tensile strength; effects of irradiation on superconducting and mechanical properties; "point defect" structure in amorphous materials using X-ray diffraction, Mössbauer spectroscopy, internal friction and position annihilation spectroscopy.

UNIVERSITY OF CALIFORNIA/DAVIS

314. RADIATION DAMAGE AND ENVIRONMENTAL EFFECTS IN NUCLEAR WASTE STORAGE MEDIA

D. G. Howitt - Dept. of Mechanical Engineering
Phone: (916)-752-1164, 0580

$ 93,000 01-1

Comparative evaluation of the response of nuclear waste storage glasses and candidate crystalline ceramics to irradiation is being studied over a range of temperatures in a variety of irradiation environments to determine the microstructural features enhancing deterioration and radiation instability in these materials. Effects of microstructural features, phase separation, precipitation, devitrification, particle size, and composite annealing temperatures on the properties of nuclear waste storage media. Numerical calculations of non-linear composition profiles in leached waste storage media. Estimation of damage cross sections for ionization and displacement processes in borosilicate glasses.

UNIVERSITY OF CALIFORNIA/DAVIS (continued)

315. DEFORMATION MECHANISMS AND FAILURE MODES IN SUPERPLASTICITY

A. K. Mukherjee - Dept. of Mechanical Engineering
Phone: (916)-752-0580

$ 81,000 (13 months) 01-2

Experimental study of superplastic deformation of metals, viz, microduplex austenitic stainless steels and Cu-base alloys; measurement of creep as a function of stress, temperature, strain rate, and microstructure, e.g., grain size; identification of controlling intragranular and intergranular creep mechanisms in alloys after various thermomechanical processing treatments; extension of above to cavitation behavior and superplastic forming limitations.

316. AN INVESTIGATION OF THE ROLE OF SINTERING IN GAS-SOLID INTERACTIONS

Z. A. Munir - Dept. of Mechanical Engineering
Phone: (916)-752-0559, 0580

$ 63,000 01-3

Investigation of the role of sintering in the kinetics of gas-solid interactions in powder compacts, including both oxidation-reduction and dissociation reactions. Study of state of division of oxide ceramics resulting from the decomposition of hydroxides and carbonates as a function of gas pressure, temperature, and impurities. Evaluation of changes of oxide particle shape and size as a function of sintering parameters. Morphological changes such as surface area, pore size, and overall porosity are measured and related to changes in the reversibility and rates of reactions. The role of sintering is elucidated by thermogravimetric, microscopy, and surface area measurement techniques.

UNIVERSITY OF CALIFORNIA/IRVINE

317. RAMAN SPECTROSCOPY OF MOLECULAR ADSORBATES

J. C. Hemminger - Dept. of Chemistry
Phone: (714)-833-6020
S. Ushioda - Dept. of Physics
Phone: (714)-833-6619

$127,000 02-2

Combine Raman spectroscopy and modern surface science technology to study binding and chemistry of adsorbates on well characterized surfaces. Study mechanism of "giant" enhanced Raman scattering. Correlate enhancement with surface roughness on stepped and kinked surface of Ag. Also correlate enhancement with electronic energy levels of metal-adsorbate system as determined by electron energy loss spectroscopy. Apply Raman spectroscopy to study of corrosion by H_2S and O_2.

318. INTERACTION OF LOW ENERGY ELECTRONS WITH SURFACE LATTICE VIBRATIONS

D. L. Mills - Dept. of Physics
Phone: (714)-833-5148

$ 94,965 02-2

Theory of electron energy loss spectroscopy (EELS) of surfaces. Vibrational properties of isolated adatoms and ordered overlayers on metal surfaces, with emphasis on quantitative comparisons with experiment. Role of image potential in large-angle EELS and in LEED studies. Large-angle inelastic scattering from substrate phonons. EELS spectral densities at large wave vector. Surface relaxation, anharmonicity, and surface lattice dynamics. This program strongly coupled to that of S. Y. Tong, University of Wisconsin-Milwaukee.

UNIVERSITY OF CALIFORNIA/LOS ANGELES

319. IRRADIATION-INDUCED PRECIPITATION AND SOLUTE SEGREGATION IN ALLOYS

A. J. Ardell - Materials Department
Phone: (213)-825-7011

$ 61,524 01-4

Irradiation-induced solute segregation and precipitation in Pd and Ni-base alloys; 20-750°C; proton, electron and heavy-ion irradiations to 0.25 dpa; effects of dose, dose rate, temperature, solute size misfit, damaging particle and alloy composition; voids; irradiation effects in metallic glasses; TEM, analytical electron microscopy and HVEM.

UNIVERSITY OF CALIFORNIA/SAN DIEGO

320. INVESTIGATION OF THE INTERACTION BETWEEN SUPERCONDUCTIVITY AND MAGNETISM AND OSCILLATORY CHEMICAL REACTIONS OVER METAL SURFACES

M. B. Maple - Dept. of Physics
Phone: (714)-452-3969

$269,239 02-2

This is an experimental research program to investigate the coexistence of superconductivity and magnetism. The primary interest is in A-15's, ternary molybdenum chalcogenides, and other high T_c superconductors. Properties of rare earth compounds such as $ErRh_4B_4$ and $ErMo_6Se_8$ will be studied in order to understand re-entrant and coexistence phenomena. Collaborative efforts to study valance instabilities in Ce compounds and the superconductivity of graphite intercalated with potassium have been initiated. A study of the oscillatory oxidation of CO on Pt using LEED and Auger techniques and a study of some metallic thin film oxidations using electrical resistance are under way.

321. RESEARCH ON THE THERMOPHYSICAL PROPERTIES OF MATERIALS

J. C. Wheatley - Dept. of Physics
Phone: (714)-452-3325

$130,112 02-5

Studies of the science of heat engines and of cryogenic materials. The following specific areas are included: (1) Intrinsically Irreversible Engines - a refrigerating acoustically driven prototype using helium-4 as the media has been developed and will be studied, (2) The further development and analysis of a liquid propylene heat pump/prime mover, (3) Thermal convection mechanisms using helium-3 = helium-4 solutions for parameter values where chaotic behavior sets in, and (4) A study of the spin alligned isotopes of hydrogen.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA

322. RESEARCH ON PHASE TRANSFORMATIONS AND NON-EQUILIBRIUM PROCESSES

J. S. Langer - Dept. of Physics
Phone: (805)-961-3495

$ 94,053 02-3

Theory of certain non-equilibrium processes of importance in design of metallurgical materials. Theory of dendritic crystal growth. Theory of eutectic solidification with emphasis on roles played by fluctuations and instabilities. Numerical and analytic studies of theory of interfacial morphology. Kinetics of phase separation in alloy solids and multicomponent fluids.

323. NUMERICAL SIMULATION OF QUANTUM MANY-BODY SYSTEMS

D. J. Scalapino - Physics Dept.
Phone: (805)-961-2871
J. R. Schrieffer - Physics Dept.
Phone: (805)-961-3061
R. L. Sugar - Physics Dept.
Phone: (805)-961-4078

$150,000 (21 months) 02-3

A program to investigate the use of stochastic numerical techniques for simulating many-body problems where the particles obey Fermi statistics. One-dimensional systems will be investigated considering various electron-phonon interactions to further the fundamental understanding of conducting polymers. One-dimensional chains of quantum mechanical spins will be studied with application to spin glasses and pseudo random spin systems such as $CeNiF_3$. Correlation effects and frequency dependent transport will be considered to test the validity of theoretical approximations such as the Padé and Padé-conformal map techniques. The program will then be extended to consider many-fermion systems in two and three spatial dimensions.

CARNEGIE INSTITUTION OF WASHINGTON

324. STUDY OF THE PROPERTIES OF HYDROGEN AT STATIC PRESSURES OF ONE MEGABAR

P. M. Bell - Geophysical Laboratory
Phone: (202)-966-0334
H. K. Mao - Geophysical Laboratory
Phone: (202)-966-0334

$ 87,000 02-2

Investigations are under way on the hydrogen isotopes, helium, neon, argon, carbon dioxide, methane and other simple gases under very high pressure. Hydrogen has been pressurized to a static pressure above 1Mbar. Laser Raman scattering studies of the molecular bonding phenomena and the elastic constants have been measured as a function of pressure to 250 kbars in hydrogen and deuterium. The Equation of State for argon has been determined to 650 kbars. Further improvement to the Diamond Anvil Cell technique is under way. The Raman and Infrared spectra of solid hydrogen will be measured to 700 kbars. Brillouin and x-ray scattering measurements on solid hydrogen and solid argon will be made to 500 kbars.

CARNEGIE-MELLON UNIVERSITY

325. CORROSION FATIGUE CRACK INITIATION UNDER PASSIVE CORROSION CONDITIONS

I. M. Bernstein - Dept. of Metallurgical Engineering and Materials Science
Phone: (412)-578-2700
A. W. Thompson - Dept. of Metallurgical Engineering and Materials Science
Phone: (412)-578-2711
G. W. Warren - Dept. of Metallurgical Engineering and Materials Science
Phone: (412)-578-3517

$ 89,800 01-2

Corrosion fatigue of austenitic stainless steels in aqueous solutions; correlation of dislocation characteristics and electrochemical parameters determining crack initiation under passive corrosion conditions; evaluation of the role of rupture processes, anodic dissolution, and hydrogen embrittlement; modelling fatigue lifetimes on a micromechanical basis.

CARNEGIE-MELLON UNIVERSITY (continued)

326. FUNDAMENTAL STUDIES OF EROSION AND EROSION/CORROSION FOR COAL GASIFICATION SYSTEMS

J. C. Williams - Carnegie Institute of Technology
Phone: (412)-578-2704
G. B. Sinclair - Dept. of Mechanical Engineering
Phone: (412)-578-2504

$ 65,000 01-5

Particulate erosion of ductile metals investigated for conditions of normal impact of rigid spherical particles and oblique impact of rigid cylindrical particles; strain distribution obtained based on the elastic-plastic behavior of metals at high strain rates; multiple impacts treated as quasi-fatigue cycles, leading to erosion loss described by a Coffin-Manson-type relationship; experiments with single and multiple particle impacts to measure substrate displacement, weight loss, and microstructural features such as crack paths and substructural changes; materials - Cu and its alloys; techniques - laser interferometry, electron microscopy.

CASE WESTERN RESERVE UNIVERSITY

327. COUPLED DIFFUSION PHENOMENA IN MULTICOMPONENT GLASSES AND GLASS FORMING LIQUIDS

A. R. Cooper - Dept. of Metallurgy and Materials Science
Phone: (416)-368-4224

$ 66,757 01-3

Study of rate processes, e.g., precipitation, dissolution and phase separation in multicomponent systems at high temperatures. Study of transport processes and thermodynamics in multicomponent molten silicate systems, and kinetics of these processes in such systems. Relation of the interdiffusion coefficient matrix to the individual ionic species mobilities or self-diffusion coefficients. Work focused on systems K_2O-SrO-SiO_2 and CaO-Al_2O_3-SiO_2. Ultimate goal is a sufficiently well-documented understanding of such transport processes that will be useful for prediction of behavior in the many high temperature processes that involve molten silicates.

CASE WESTERN RESERVE UNIVERSITY (continued)

328. FUNDAMENTAL STUDIES OF STRUCTURE-PROPERTY RELATIONSHIPS IN TRANSFORMATION-TOUGHENED CERAMICS

A. H. Heuer - Dept. of Metallurgy and Materials Science
Phone: (216)-368-3868

$134,555 01-2

Ostwald ripening in ZrO_2 toughened Al_2O_3. Plastic deformation in two phase "single crystal" partially-stabilized ZrO_2, and in 100% tetragonal ZrO_2 polycrystals. The focus of these studies will be the nature and extent of the transformation zone associated with propagating cracks and the critical factors involved in processing strong and tough polycrystalline tetragonal ZrO_2.

UNIVERSITY OF CHICAGO

329. RESEARCH IN THE THEORY OF CONDENSED MATTER AND ELEMENTARY PARTICLES

L. P. Kadanoff - The James Franck Institute
Phone: (312)-962-7189
Y. Nambu - The James Franck Institute
Phone: (312)-962-7286

$138,157 02-3

Theoretical research on problems relevant to both elementary particle physics, through quantum field theory, and condensed matter physics, via the statistical mechanics of phase transitions. Topics of current interest include: non-linear dynamical systems and the transition to chaos, dendritic growth, parallel processing computers as statistical mechanical systems, chiral symmetry breaking in lattice gauge theories, quantized string theory (free and interacting), and problems of chiral fermions in lattice theories.

CLARK COLLEGE

330. STUDY OF CHARGE TRANSPORT IN THE THERMOELECTRET STATE OF SOME CERAMICS AND GLASSES

O. P. Puri - Dept. of Natural Sciences and Mathematics
Phone: (404)-681-3080 x200

$ 70,000 01-3

Investigation of the mechanism of formation and decay of electrets in non-polar inorganic polycrystalline and amorphous dielectrics. Experimental characterization of electret formation with sample temperature, polarization field, and cooling rate, and of electret decay in the open and closed circuit condition. Extension of Swann-Gubkin theory by considering the non-polar part of electret polarization through the displacement of ions to account for the production of non-polar electrets. Materials of interest include $CaTiO_3$, $SrTiO_3$, $BaO \cdot 4TiO_2$, $BiTiO_3$, $(SrBi)TiO_3$, chalcogenide glasses and elemental Se. X-ray diffraction. Thermally stimulated discharge current analysis.

COLORADO SCHOOL OF MINES

331. FERROUS ALLOY METALLURGY - LIQUID LITHIUM CORROSION AND WELDING

D. Olson - Dept. of Metallurgical Engineering
Phone: (303)-273-3787
D. Matlock - Dept. of Metallurgical Engineering
Phone: (303)-273-3775

$152,000 01-5

Range of austenite phase stability in Fe-Ni-Cr and Fe-Ni-Mn weld filler metals with various additions (Al, Cu, Mo, Nb, Si, Ti, W, C and N); thermal expansion coefficients for these alloys; weld metal solidification and its relation to solute partitioning; impression creep of weldments, initially of Al and of dissimilar steels; role of microchemistry and structure on weld mechanical properties; dissimilar welds in 2¼ Cr-1 Mo /316 stainless steel; gas metal arc weld strip overlay cladding process. Dissolution kinetics of austenitic stainless steels in molten Li; corrosion fatigue and embrittlement of ferritic steels in molten Li.

UNIVERSITY OF COLORADO

332. LIGHT SCATTERING STUDIES OF LOWER DIMENSIONAL COLLOIDAL PARTICLE AND CRITICAL FLUID SYSTEMS

W. O'Sullivan - Dept. of Physics
Phone: (303)-492-7457
R. Mockler - Dept. of Physics
Phone: (303)-492-8511

$188,000 (18 months) 02-2

Using a variety of laser light scattering and optical microscopy techniques study lower dimensional behavior. Answer fundamental questions concerning the universality of fluid dynamical critical behavior in two dimensions. Effects of reduced dimensionality on melting of charged colloidal particle suspensions (CCPS) crystals, on supercooling of CCPS liquids and the response of CCPS crystals to transient electric fields. Dynamic critical properties of thin film fluid films. Study physics of crystalline state and liquid state colloidal particle monolayers formed on liquid surfaces and membranes.

COLUMBIA UNIVERSITY

333. DEFECT INTERACTIONS AT HIGH CONCENTRATIONS IN SOLID OXIDE ELECTROLYTES

A. S. Nowick - Krumb School of Mines
Phone: (212)-280-2921

$ 79,410 01-3

Interactions of defects at high concentrations in oxides that are fast-ion conductors; CeO_2 doped with Y and Sc; study of relationship between defect structure, electrical properties, and grain boundary microchemistry; relationship between simple defects that form at low concentrations and the ordering and microdomain formation observed at high concentrations; kinetics of cationic ordering. Defect energy calculations. Complex impedance plots and the "grain-boundary effect." Ordering studies as a function of ionic radius difference between M^{3+} and host cation, initially for $Zr_3Er_4O_{12}$. Analytical electron microscopy of grain boundary microchemistry. Anelastic relaxation-internal friction. Neutron scattering. Ionic thermo-current dielectric relaxation defect studies. Synchrotron EXAFS experiments on $CeO_2:Y_2O_3$ solid solutions at the Brookhaven National Synchrotron Light Source.

UNIVERSITY OF CONNECTICUT

334. ELECTRODE POLARIZATION STUDIES IN HOT CORROSION SYSTEMS

O. F. Devereux - Dept. of Metallurgy
Phone: (203)-486-4714

$ 73,000 01-3

Electrode polarization behavior of Ni in molten salts based on either Na_2CO_3 or FeS + Na_2S; anodic and cathodic half cell reactions identified at various O:S activities in the electrolyte; mechanisms of corrosion; kinetics of sulfidation of Fe measured in gaseous environments.

335. ENERGY TRANSFER AND NON-LINEAR OPTICAL PROPERTIES AT NEAR ULTRA-VIOLET WAVELENGTHS: RARE EARTH 4f → 5d TRANSITIONS IN CRYSTALS AND GLASSES

D. Hamilton - Dept. of Physics
Phone: (203)-486-3856

$ 46,704 02-2

Investigation of non-linear optical transitions and inter-ionic energy transfer in the near UV 5d electronic states of rare earth impurity-doped crystals and glasses. Dynamic polarization spectroscopy (DPS) used as a primary technique. Other nonlinear and multiphoton spectroscopic methods also used as needed for more complete determination of the nature of the 5d orbitals.

336. THE FATIGUE BEHAVIOR OF 9- AND 12 Cr FERRITIC STEELS AT ELEVATED TEMPERATURE

A. J. McEvily - Metallurgy Dept.
Phone: (203)-486-2941

$ 57,000 01-2

Creep-fatigue behavior of ferritic steels (9-12% Cr) related to micro-structural features (grain size, carbide distribution, bainitic vs martensitic structure), oxidation resistance, fracture mechanics parameters, and fabrication (wrought vs welded condition); creep crack growth modelling for ductile alloys.

UNIVERSITY OF CONNECTICUT (continued)

337. INVESTIGATION OF ROLE OF SUBSURFACE ZONES IN WEAR OF MATERIALS

S. Rice - Dept. of Mechanical Engineering
Phone: (203)-486-2153

$ 89,500 01-5

Experimental characterization of the formation, composition and morphology of both subsurface zones and wear debris for material pairs making solid contact both in sliding and repetitive impact modes; experimental investigation of the roles of nominal contact stress, relative sliding velocity and effective contact stiffness of subsurface zone formation, composition and morphology; analytical prediction of the equilibrium configuration of subsurface morphology for a work hardening elastoplastic material subject to given load cycling and temperature distributions; model development which allows prediction of composition and morphology of subsurface zones for selected materials subjected to both sliding and impulsive contact; and postulation and experimental investigation of in situ development of wear resistance.

CORNELL UNIVERSITY

338. INFLUENCE OF GRAIN BOUNDARIES ON THE ELECTRICAL TRANSPORT PROPERTIES OF POLYCRYSTALLINE SI FILMS

D. G. Ast - Dept. of Materials Science and Engineering
Phone: (607)-256-4140

$ 92,900 01-1

Characterization of the structure and electrical activity of defects in hot pressed and annealed Si bicrystals; examination of coherent and asymetric twins, and tilt and twist boundaries; relationship of boundary structure to annihilation of minority carriers and in turn to electrical activity of the Si; techniques used: HVEM, TEM, electron beam induced charge in SEM.

CORNELL UNIVERSITY (continued)

339. INITIAL STAGES OF OXIDATION OF METALS

J. M. Blakely - Dept. of Materials Science and Engineering
Phone: (607)-256-5149

$139,700 (23 months) 01-1

Relationship of structure of BeO surface films to growth kinetics and to the Be substrate morphology; effect of Ni-Fe substrate composition and surface segregation of solutes on oxide characteristics; influence of sulfur containing gases and surface modification on oxidation; transition from thin to thick oxide film; techniques used: AES, UPS, EELS, LEED.

340. MIGRATION OF GRAIN BOUNDARIES IN CERAMIC MATERIALS WITH PARTICULAR REFERENCE TO THE SINTERING PROCESS

C. B. Carter - Dept. of Materials Science and Engineering
Phone: (607)-256-4797

$ 93,500 01-1

Study of the effect of geometry and composition of interfaces on interfacial mobility in ionic and covalent solids. Concerns include (1) misorientation between grains and boundary plane orientation, (2) geometry to interfacial dislocations and steps, (3) interfacial chemistry including local segregation and non-stoichiometry, and (4) interfacial pinning by pores or crystalline or amorphous pockets or films of a second phase. Materials of investigation include Al_2O_3, MgO, NiO, Mg-Al spinel, Si, and Ge. Studies on both powder compacts and bicrystals involve visible light microscopy, electron microprobe analysis, and strong- and weak-beam, lattice fringe, X-ray energy dispersive, and electron energy loss TEM analysis.

CORNELL UNIVERSITY (continued)

341. MECHANICAL PROPERTIES OF CRYSTALLINE SOLIDS

Che-Yu Li - Dept. of Materials Science and Engineering
Phone: (607)-256-4349
S. Mukherjee - Dept. of Theoretical and Applied Mechanics
Phone: (607)-256-7143

$190,000 01-2

The research includes the development of a state variable approach for the description of the mechanical properties of crystalline solids. An important objective of the work is the development of useful methods for materials testing and characterization and for stress analysis and mechanical design. Specific topics are the effects of thermal and mechanical history, deformation related phenomena, microstructure based theories, fundamental research on numerical methods and applications to complex technological problems.

342. PROBABILISTIC MODELS OF THE STRESS-RUPTURE OF COMPOSITE MATERIALS

S. L. Phoenix - Sibley School of Mechanical and Aerospace Engineering
Phone: (607)-256-3462

$ 95,000 01-2

Modelling tensile and stress rupture strengths of fiber reinforced polymer composites based on a probabilistic statistical representation of the measured distribution of fiber strengths; development of relationships between the strength and lifetime of Kevlar fibers, fiber epoxy strands, and composite pressure vessels; influence of initial fiber breaks on composite time to failure; development of asymtotic analyses and application of these to the tensile strength of composites with different shapes and load sharing rules; extension of tensile results to 3D composites; effect of matrix viscoelasticity on creep and stress rupture for carbon, S-glass, and Kevlar fibers in polyester and epoxy matrices.

CORNELL UNIVERSITY (continued)

343. HIGH TEMPERATURE MECHANICAL BEHAVIOR OF SILICON NITRIDE

R. Raj - Dept. of Materials Science and Engineering
Phone: (607)-256-4040

$117,000 (17 months) 01-2

Creep cavitation in ceramics under multiaxial loading and densification mechanisms in ceramics in the hot isostatic pressing process. In-situ measurements of densification rate of powder compacts under a variable confining pressure.

344. DIFFRACTION AND MICROSCOPY STUDIES OF THE STRUCTURE OF GRAIN BOUNDARIES IN Fe, Fe-BASE ALLOYS, AND CERAMIC MATERIALS

S. L. Sass - Dept. of Materials Science and Engineering
Phone: (607)-256-5239

$149,000 01-1

Investigation of grain boundary structure of metals and ceramics using TEM and x-ray diffraction; tilt boundary dislocation structure in NiO; modelling diffraction from grain boundary regions to indicate lattice dilation there.

DARTMOUTH COLLEGE

345. THE ROLE OF GRAIN SIZE ON THE BRITTLE TO DUCTILE TRANSITION OF THE STRONGLY ORDERED ALLOY Ni_3Al

E. M. Schulson - Thayer School of Engineering
Phone: (603)-646-2888

$ 88,100 01-2

Characterization of Ni_3Al powder produced by rapid solidification; consolidation by extrusion; measurement and correlation of grain size and dislocation structure with mechanical behavior, e.g., yielding, work hardening, and creep; use of SEM to evaluate fracture morphology and AES to examine impurity segregation to grain boundaries.

UNIVERSITY OF DELAWARE

346. ANALYSES OF FAILURE MODES IN SHORT FIBER REINFORCED THERMOPLASTICS

T. W. Chou - Dept. of Mechanical and Aerospace Engineering
Phone: (302)-738-2904

$ 60,000 01-2

Calculation of physical and mechanical properties of polymers reinforced with discontinuous fibers; strength and strain hardening found for the parallel fiber case using variational and statistical methods; measurement of strength distribution of carbon and glass fibers (sometimes with prestressing) and of composites containing these; relationship of composite failure mode to fiber type and volume fraction.

UNIVERSITY OF DENVER

347. THE DETECTION OF HYDROGEN ASSISTED CRACK GROWTH

S. H. Carpenter - Dept. of Physics
Phone: (303)-753-2176

$ 72,500 01-5

Experimental investigation of H_2 induced deformation and cracking in steels; measurement of kinetics of cracking during exposure to H_2 with and without applied stress; influence of vacuum annealing on crack healing; techniques used--acoustic emission, modulus defect.

348. THERMAL EXPANSION EFFECTS IN CORDIERITE

P. K. Predecki - Dept. of Chemistry
Phone: (303)-753-2141

$ 80,000 01-3

Effect of solid solutions of various sized ions in cordierite on thermal expansion. Solutes considered are Ge, B and P substituted on tetrahedral sites, Zn and Li substituted on octahedral sites, and alkali and alkaline earth ions interstitially in the large C-axis channels. Measurement of lattice thermal expansion coefficient on powder samples over the range from 25° to 800°C by X-ray diffraction using a Huber-Guinier high-temperature counter-based diffraction system equipped with computer control and handling of data by a Nicolet Dual L-11 system. Correlation of lattice thermal expansion with both lattice distortion and changes with X-ray diffracted intensity. Ultimate objective is to understand how changes in substitutional and interstitial lattice site occupancy and associated local bond distortions affect the lattice expansion coefficients.

EMORY UNIVERSITY

349. FAR INFRARED STUDIES OF SUPERCONDUCTING V_3Si, Nb_3Ge, AND Nb

S. Perkowitz - Physics Dept.
Phone: (404)-329-6584

$ 43,901 02-2

Optical techniques in the far infrared region will be used to explore the basic superconducting behavior of the high temperature superconductors V_3Si, Nb_3Ge, Nb and granular NbN. Such spectroscopy will yield accurate gap values, information about the temperature dependence of superconducting properties, values of the electron-phonon spectral function and insight into grain-to-grain coupling in inhomogeneous geometries. These results will be used to calculate basic superconducting parameters such as the coupling constant and the transition temperature, T_c, with the aim of explicating the underlying physics of superconductors.

FLORIDA STATE UNIVERSITY

350. POLYMERS IN MECHANOCHEMICAL SYSTEMS: STRUCTURE-PROPERTY REQUIREMENTS

L. Mandelkern - Dept. of Chemistry
Phone: (904)-644-2054

$101,845 (24 months) 03-1

Studies on the influence of the lamellar, interfacial and interlamellar structures on the fundamental mechanical properties of polymers. Preparation of mixtures of molecular weight fractions of linear polyethylene to acquire a wide range of crystalline morphologies and crystallization of molecular weight fractions of linear polyethylene from a range of dilute to concentrated solutions. Studies will be performed on the mechanical behavior of a set of copolymers of varying co-unit concentration to compliment work on copolymers and branched polymers.

UNIVERSITY OF FLORIDA

351. METAL DISSOLUTION KINETICS IN ORGANIC SOLVENTS USING ROTATING RING-DISC VOLTAMMETRY

J. R. Ambrose - Dept. of Materials Science and Engineering
Phone: (904)-392-1456

$90,000 (24 months) 01-3

Characterization of electrochemistry of Ni-base binary alloys in alcohol solutions of Fe-base binary alloys in aqueous solutions; measurement of metal dissolution kinetics using rotating ring-disc voltammetry; identification of dominant processes of film formation and corrosion.

352. SYNTHESIS AND PROPERTIES OF WATER-SOLUBLE COPOLYMERS AND OTHER POLYMERS OF DEFINED STRUCTURE

T. E. Hogen-Esch - Dept. of Chemistry
Phone: (904)-392-2011
G. B. Butler - Dept. of Chemistry
Phone: (904)-392-2012

$ 85,000 03-1

Synthesis and characterization of water-soluble polymers and other polymer analogs of interest in enhanced oil recovery. Relaxation studies will be related to various rheological properties such as shear dependent viscosity, shear degradation and drag reduction.

UNIVERSITY OF FLORIDA (continued)

353. LOW AND MODERATE TEMPERATURE OXIDATION OF ATOMICALLY CLEAN NICKEL, CHROMIUM AND Ni-Cr ALLOYS

P. Holloway - Dept. of Materials Science and Engineering
Phone: (904)-392-1461
C. Batich - Dept. of Materials Science and Engineering
Phone: (904)-392-1461

$110,000 01-3

Investigation of low and moderate temperature (100 K < T < 800 K) oxidation of atomically clean single and polycrystalline Ni, Cr and Ni-Cr alloys is proposed. Surface segregation studies by Auger electron, x-ray photoelectron and ion scattering spectroscopies. Oxidation kinetics and adsorbed states characterization in ultra-high vacuum (UHV) with x-ray photoelectron spectroscopy, scanning Auger electron spectroscopy, low energy and reflection high-energy electron diffraction (LEED and RHEED), work function changes and temperature desorption spectroscopy. Oxide structure analysis with LEED, RHEED and transmission electron microscopy. The oxygen pressure will be varied from 10^{-10} Torr to 1 atmosphere, with higher pressure exposures being accomplished in a reaction chamber external to the UHV chamber. Specific aspects of the oxidation to be studied include oxide nucleation, lateral oxide growth to form a coalesced layer, thickening of the coalesced oxide layer, dissolution of the oxygen into the bulk and the effect of controlled oxide microstructure upon high temperature oxidation. This study will directly investigate the phenomena occurring in the transition from an atomically clean surface to a thick oxide at elevated temperatures.

354. FIELD-ION MICROSCOPY AND SPECTROSCOPY OF HYDROGEN IN METALS

J. J. Hren - Dept. of Materials Science and Engineering
Phone: (904)-392-1456

$ 76,300 01-3

Investigation of hydrogen trapping sites and diffusion in BCC and FCC metals (Nb and Ni, respectively) using TEM and field ion microscopy; pulse desorption to determine trap site energetics; influence of substitutional solutes on above.

THE FRANKLIN INSTITUTE

355. PHYSICS OF HIGHLY ANISOTROPIC MATERIALS

Siu-Tat Chui - Physics Dept.
Phone: (302)-738-8115

$ 24,000 02-3

Theoretical research focused on instabilities and elementary excitations associated with correlations in highly anisotropic (mainly quasi-one-dimensional) materials. Principal subject areas include: spin and charge density wave relationships, correlations in half filled bands, solitons and Hubbard model excitations, and superconductivity in one-dimensional systems.

GEORGIA INSTITUTE OF TECHNOLOGY

356. THE STRUCTURE AND REACTIVITY OF HETEROGENEOUS SURFACES AND STUDY OF THE GEOMETRY OF SURFACE COMPLEXES

U. Landman - School of Physics
Phone: (404)-894-3368

$149,250 02-3

Theoretical studies of surface phenomena aimed toward fundamental understanding of processes which govern the properties of material surfaces. Areas included cover surface reactivity, surface crystallography, electronic and vibrational structure, dynamical processes, phase transformations and phase changes and the properties of interfaces. Surface melting and solidification have been of high current interest. Also included are studies of surface defects, heterogeneities and reaction mechanisms.

HARVARD UNIVERSITY

357. DRIFT MOBILITIES BY TIME OF FLIGHT METHODS AND TIME DEPENDENT PHOTOTRANSPORT IN THE NANOSECOND REGIME IN AMORPHOUS SEMICONDUCTORS

W. Paul - Div. of Applied Sciences
Phone: (617)-495-2853

$105,000 02-2

Transport properties of amorphous semiconductors will be determined by measurements of drift mobilities by time of flight methods and time dependent phototransport in the nanosecond regime. Correlations with characterization and physical property measurements will be made on carefully prepared samples. Computer modeling studies may be undertaken.

HARVARD UNIVERSITY (continued)

358. FUNDAMENTAL PROPERTIES OF SPIN-POLARIZED QUANTUM SYSTEMS

I. F. Silvera - Dept. of Physics
Phone: (617)-495-2872

$260,000 (18 months) 02-2

A program to experimentally investigate the properties of the quantum gases of spin-polarized atomic hydrogen and deuterium. A major effort will be to attempt to reach high enough densities and low enough temperature that these unusual gases will experience Einstein-Bose Condensation. If this new form of matter is reached, the expected superfluidity of this weakly interacting gas will be sought and, if found, investigated.

UNIVERSITY OF ILLINOIS/CHICAGO CIRCLE

359. OXIDATION OF TRANSITION METALS IN CHLORINE CONTAMINATED ENVIRONMENTS

M. McNallen - Dept. of Materials Engineering
Phone: (312)-996-2436

$ 30,800 (17 months) 01-3

Experimental investigation of the oxidation of metals (Fe, Co, Ni) in mixed gas (O_2-Cl_2) environments; thermogravimetric measurement of corrosion kinetics.

UNIVERSITY OF KENTUCKY

360. STUDIES OF THE MICROSCOPIC PHYSICAL AND CHEMICAL PROPERTIES OF GRAPHITE INTERCALATION COMPOUNDS

P. C. Eklund - Dept. of Physics and Astronomy
Phone: (606)-257-6725

$100,035 02-2

Experimental research on graphite intercalation compounds, especially with antimony halide and alkali metal intercalates. Techniques include optical reflectance (infrared to VUV), Raman scattering, Mossbauer spectroscopy, x-ray diffraction, neutron scattering, and magnetoresistance.

361. ANISOTROPIC ELASTICITY OF COAL

P. P. Gillis - Dept. of Metallurgical Engineering and Materials Science
Phone: (606)-257-5733, 8883
A. B. Szwilski - Dept. of Civil Engineering
Phone: (606)-257-2953, 4856

$ 89,000 01-2

Investigations of the anisotropic elastic constants of coal. Static and dynamic measurements are performed and attempts to relate the results to the structure of the various coals being studied are being made. Objectives include the development of coal-sample preparation/selection procedures that lead to meaningful and reproducible research results.

362. STRUCTURAL CHARACTERIZATION OF DISPERSED METAL CATALYSTS

P. J. Reucroft - Dept. of Metallurgical Engineering and Materials Science
Phone: (606)-257-8723
R. J. De Angelis - Dept. of Metallurgical Engineering and Materials Science
Phone: (606)-257-3238

$ 94,000 (16 months) 03-3

Correlation of catalyst activity in hydrogenation reactions to the structure and morphology of the active and support phases; active phase-Ni with solutes of high oxidizing potential;support phase - SiO_2, $MgSiO_3$; techniques used: TEM, X-ray scattering.

LEHIGH UNIVERSITY

363. AN EXPERIMENTAL AND ANALYTICAL INVESTIGATION OF THE CREEP-RUPTURE PROCESS

T. Delph - Dept. of Mechanical Engineering and Mechanics
Phone: (215)-861-4119

$ 60,695 01-2

Experimental and modelling study of creep in austenitic stainless steels under uniaxial and multiaxial stress states; measurement of cavitation and precipitation kinetics with SANS; analysis of cavity linkage.

364. ELECTRON-OPTICAL AND MICROANALYTICAL STUDIES OF PRECIPITATION IN CERAMIC SYSTEMS

M. R. Notis - Materials Research Center
Phone: (215)-861-4225
D. B. Williams - Materials Research Center
Phone: (215)-861-4225
M. P. Harmer - Materials Research Center
Phone: (215)-861-4225

$120,000 01-1

Study of precipitation phenomena by means of analytical and high resolution electron microscopy. Phase transformation resulting in transformation toughening in ZrO_2 containing ceramics. Precipitate dissolution kinetics and transient second phase phenomena. Precipitate coarsening kinetics in NiO and CoO, and precipitation processes in mullite and ceramic glazes.

365. MECHANICS AND CHEMISTRY OF SMALL CRACKS IN CORROSION FATIGUE

R. P. Wei - Dept. of Mechanical Engineering and Mechanics
Phone: (215)-861-3587

$ 90,000 (13 months) 01-2

Experimental and theoretical study of corrosion fatigue of steels in aqueous solutions; small fatigue crack growth kinetics as a function of frequency, environment and crack length; modelling of electrochemical conditions near the crack tip and of the micromechanics of small crack growth.

LOUISIANA STATE UNIVERSITY

366. STUDIES OF SUB-MICRON DEVICES WITH EMPHASIS ON MOS SYSTEMS

R. F. O'Connell - Dept. of Physics and Astronomy
Phone: (504)-388-6835

$ 62,001 02-3

Theoretical study of electrons in quasi-two-dimensional systems, as relevant to the physics of sub-micron devices. Magneto-optical phenomena in metal-oxide-semiconductor (MOS) systems. Wigner distribution function (WDF) techniques in sub-micron device physics. Strong magnetic and electric field effects in two-dimensional systems.

UNIVERSITY OF MARYLAND

367. ADSORPTION ON METAL SURFACES

T. L. Einstein - Dept. of Physics
Phone: (301)-454-3419
R. E. Glover, III - Dept. of Physics
Phone: (301)-454-3417
R. L. Park - Dept. of Physics
Phone: (301)-454-4126

$175,000 02-2

Joint theoretical/experimental study of surface interactions which, though they involve small characteristic energies, have a significant influence on surface reactivity. Investigation of the molecular precursor state of oxygen on thin film and fully-characterized single crystal metal surfaces; identification of the physical nature of the activation barrier. Study of adatom-adatom interactions using high-resolution LEED/Auger to examine long- and short-range order of chemisorbed layers; Monte-Carlo simulations of phase diagrams will be made to obtain interaction parameters. Experimental determinations of critical exponents associated with two-dimensional phase transitions and comparison with phase-transition theory.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

368. MICROMECHANICAL MODELLING OF MICROSTRUCTURAL DAMAGE AT ELEVATED TEMPERATURE DURING CREEP OF SUPERALLOYS FOR ENERGY APPLICATIONS

A. S. Argon - Dept. of Mechanical Engineering
Phone: (617)-253-2217
F. A. McClintock - Dept. of Mechanical Engineering
Phone: (617)-253-2219

$130,000 01-2

Analysis of creep cavitation and cracking in metals--Cu, Ni-base alloys, and austenitic stainless steels; stress and strain concentrations at particles on grain boundaries modelled and their influence on local deformation and cavitation assessed; calculation of cavity growth in diffusion vs deformation controlled strain fields; relaxation processes around a macroscopic crack tip; measurement of crack growth in steels and of cavity growth kinetics under multiaxial stress states in Cu.

369. STRUCTURE AND PROPERTIES OF GRAIN BOUNDARIES

R. W. Balluffi - Dept. of Materials Science and Engineering
Phone: (617)-253-3349
P. D. Bristowe - Dept. of Materials Science and Engineering
Phone: (617)-253-3326

$311,269 01-1

Grain boundaries in metals and ceramics; experimental, theoretical and computer simulation; computer simulation of intrinsic structures of grain boundaries and grain boundary dislocations; computer simulation of the structure and energy of point defects in grain boundaries; investigation of various grain boundary models using computer simulation and physical modeling; effect of thermal energy on grain boundary structure and diffusional processes; experimental study of relationship between the energy of crystalline interfaces and their crystal misorientation; mechanisms for grain boundary migration.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

370. INTERFACIAL AND COLLOIDAL ASPECTS OF AQUEOUS SUSPENSIONS CONTAINING OXIDIC POWDERS

A. Bleier - Dept. of Materials Science and Engineering
Phone: (617)-253-6877

$95,000 (15 ½ months) 01-5

Application of colloid-chemical models of single and multimetallic oxides to the processing of their powders. Extension of such models to heterogeneous systems containing more than one particle (composition) type, so as to improve understanding of interfacial complexation and related phenomena which influence dispersibility and packing behavior. Objectives include preparation of model, colloidal single and multimetallic oxides using established synthesis routes, characterization of these oxides using crystallographic, chemical, physical, and surface-chemical procedures, and evaluation of the Davis, James, and Leckie model of the electrical double layer.

371. PHYSICS AND CHEMISTRY OF PACKING FINE CERAMIC POWDERS

H. K. Bowen - Dept. of Materials Science and Engineering
Phone: (617)-253-6892

$112,000 01-5

Development of a scientific basis for the processing and packing behavior of the model sub-micron ceramic powders SiO_2, TiO_2, and SiC. Synthesis aspects of colloid chemistry and mono-sized particle masses. Colloid coagulation. Surface chemistry and powder characterization. Ordering behavior of particulate assemblies. Effects of particle size distribution on slurry stability. Dispersion, packing, and sintering behavior. Generalizations controlling the presintered structure of compacts containing $\sim 10^{12}$ particles.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

372. MODIFICATION OF THE PROPERTIES OF BENZENE-DERIVED GRAPHITE FIBERS BY INTERCALATION AND IMPLANTATION

M. S. Dresselhaus - Center for Materials Science and Engineering
Phone: (617)-253-6864
G. F. Dresselhaus - Center for Materials Science and Engineering
Phone: (617)-253-6827

$130,000 (24 months) 02-2

A comprehensive study of the structure and property relationships of benzene-derived fibers, both in their pristine form and as modified by intercalation and implantation will be undertaken. Preliminary studies of these fibers has found structural, mechanical and electrical properties approaching those of graphite single crystals--superior to those of fibers formed by other techniques. Emphasis will be given to characterization by high resolution TEM studies to identify defects introduced by intercalation and implantation.

373. IRRADIATION MICROSTRUCTURES IN NUCLEAR CERAMICS FOR FUSION ENERGY AND NUCLEAR WASTE DISPOSAL

L. W. Hobbs - Ceramics and Materials Science Dept.
Phone: (617)-253-6835

$134,000 01-4

Characterization of irradiation stability and radiation damage microstructures of crystalline ceramic solids and applications to radioactive waste containment. Microstructural origins of radiation-induced degradation and swelling. Irradiation responses to be investigated include point defect aggregation, phase instability, precipitation, decomposition and the crystal→glass (metamict) transformation. Accelerated irradiation is to be provided through use of fast neutrons, heavy ions, α-emitting dopants, and in certain cases (very light elements or where radiolytic damage mechanisms exist) fast electrons. Previously irradiated materials are also available for examination. Transmission electron microscopy including high-resolution structure imaging methods and scanning TEM (STEM) analytical techniques. Facilities are additionally available for examining highly-radioactive samples containing actinides. Materials to be examined include: BeO; the fluorite oxides $(Zr,Y)O_2$, PuO_2 (and the prototype fluorite CaF_2); the lithium breeder compounds Li_2O, $LiAlO_2$, Li_2ZrO_3; three non-oxide ceramics AlON, Si_3N_4, SiC; SiO_2, GeO_2 and simple silicates; the SYNROC phases $CaZrTi_2O_7$, $BaAl_2Ti_6O_{16}$; and actual PUREX waste solidified by the Sandia process.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

374. BASIC RESEARCH IN CERAMIC SYSTEMS

W. D. Kingery - Dept. of Materials Science and Engineering
Phone: (617)-253-3319
R. L. Coble - Dept. of Materials Science and Engineering
Phone: (617)-253-3318

$650,000 01-1

Electrical and optical behavior of Al_2O_3 and MgO, float zone crystal growth and zone refining of Al_2O_3, and grain boundary migration in high purity powder and bicrystals of Al_2O_3. Kinetic studies including oxygen diffusion in single crystal and deformed MgO, reaction processes and microstructure development in low temperature sub-solidus systems, influence of boundary segregation on grain boundary diffusion in MgO. Defect and grain boundary structures and interactions including non-ohmic conduction at grain boundaries in semiconducting oxides, grain boundary segregation in Al_2O_3 and MgO, electrical properties of grain boundaries in MgO, defect structure in single crystal ZnO, defect structure and complex ions at grain boundaries and surfaces, effects of silica doping on $SrTiO_3$ capacitors and ZnO varistors, and non-stoichiometry in SiC. Sintering related studies include powder preparation and sintering of Al_2O_3, grain boundary migration in alkali halides, recrystallization and creep in the W-Ni system, diffusion induced grain boundary migration and discontinuous precipitation, Co segregation at WC grain boundaries, and grain boundary: solid vapor configuration experiments. Powder preparation. Ceramic technology transfer and technology interchange.

375. IMPROVEMENT IN HIGH MAGNETIC BEHAVIOR OF VANADIUM-GALLIUM SUPERCONDUCTORS BY ENHANCEMENT OF SPIN ORBIT SCATTERING

R. H. Meservey - Francis Bitter National Magnet Laboratory
Phone: (617)-253-5578
P. M. Tedrow - Francis Bitter National Magnet Laboratory
Phone: (617)-253-5578

$101,800 (9 months) 02-2

The A15 compound V_3Ga is the best known superconducting material for the fabrication of practical high field magnets. Its usefulness is, however, restricted to about 25T. This is believed to be due to the low spin-orbit scattering because of the low Z elemental components. Two approaches to increasing the spin-orbit scattering will be taken by this program--the inclusion of randomly placed high Z elements with minimum lattice distortion and thin closely spaced high Z material layers. Samples will be prepared by electron beam evaporation and characterized by the superconducting properties, resistivity and spin-polarized tunneling measurements. These measurements will test existing theoretical concepts and are expected to advance the understanding of high field superconductors as well as the role of many-body effects in normal transition metallic systems and the development of improved magnetic solenoids.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

376. TRANSFORMATION PLASTICITY IN HIGH-STRENGTH MATERIALS

G. B. Olson - Dept. of Materials Science and Engineering
Phone: (617)-253-6901
I. W. Chen - Dept. of Materials Science and Engineering
Phone: (617)-253-7100
A. S. Argon - Dept. of Materials Science and Engineering
Phone: (617)-253-2217

$100,500 01-2

Development of constitutive flow relations for transformation plasticity in metals (austenitic, martensitic, and low alloy steels), ceramics (ZrO_2, HfO_2, and model alkali halides), and amorphous metals (Co-based) based on local deformation mechanisms; correlation of flow behavior with martensitic transformation kinetics, influence of stress state on transformation plasticity; deformation and microcracking processes accommodating transformation strains; techniques used--TEM, x-ray diffraction, saturation magnetization.

377. LOW TEMPERATURE AND NEUTRON PHYSICS STUDIES

C. G. Shull - Dept. of Physics
Phone: (617)-253-4812

$280,189 02-1

Fundamental experiments in neutron diffraction and interferometry using the MIT research reactor, such as the analogue of the famous optical Fizeau experiment in which fringe shifts are observed when light is sent through a moving medium; neutrons entering a crystal at an exact Bragg angle propagate through the crystal along the Bragg planes at a drift velocity much less than the group velocity. Ways are sought to exploit this effect. Ways are also sought to use neutron interferometry to test nonlinear variants of wave mechanics. Effect of interferometer rotation; nature of coherent wave front in interferometer; single and multiple slit Fresnel diffraction patterns.

378. A BASIC STUDY OF HEAT FLOW IN FUSION WELDING

J. Szekely - Dept. of Materials Science and Engineering
Phone: (617)-253-3236
T. Eagar - Dept. of Materials Science and Engineering
Phone: (617)-253-3229

$ 48,164 01-5

Modelling of arc welding processes; effect of spatial distribution of the heat source, e.g., point vs line, on the weld penetration and the heat affected zone width; plasma temperature and velocity profiles; weld pool shape; corroborative experiments; material-low alloy steels.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

379. FUNDAMENTAL INVESTIGATIONS OF THE OXIDATION OF ALLOYS IN MULTICOMPONENT GASEOUS ENVIRONMENTS

G. J. Yurek - Dept. of Materials Science and Engineering
Phone: (617)-253-3239

$128,400 01-3

Oxidation of Cr, Fe-Al, and Fe-Cr in gases with a range of O:S activities; differences in Cr_2O_3 formation kinetics and structure depending upon substrate crystallographic orientation; effect of CrS non-stoichiometry on oxide-sulfide boundary on stability diagrams; mechanisms controlling scale growth; comparison of corrosion behavior of conventional and rapidly solidified materials.

UNIVERSITY OF MASSACHUSETTS

380. SYNTHESIS OF METASTABLE SUPERCONDUCTING COMPOUNDS BY ION IMPLANTATION AND ELECTRON BEAM MELTING AND SPIN QUENCHING

M. T. Clapp - Dept. of Mechanical Engineering
Phone: (413)-545-0868

$ 45,739 02-2

Use of ion implantation and spin quenching to form metastable A-15 and amorphous superconducting materials. Ion implantation used both to optimize stoichiometry and to introduce selected impurities. Spin quenching used as a rapid solidification technique for amorphous materials. Furnace and electron beam annealing used to remove radiation damage in implanted samples and to crystallize amorphous preparations. Current interests: Nb_3Al, implanted with B and C; Nb_3Si and Nb_3Ge, implanted with C, N, and O.

381. EROSION OF STRUCTURAL CERAMICS

J. E. Ritter, Jr. - Dept. of Mechanical Engineering
Phone: (413)-545-0632, (413)-235-2414
K. Jakus - Dept. of Mechanical Engineering
Phone: (413)-545-2424

$ 38,570 01-5

Erosion behavior and related strength degradation of Al_2O_3, Si_3N_4, and SiC at temperatures to 1200°C. Assessment of erosion models for predicting erosion behavior and associated strength degradation. Effect of eroding particle velocity, size, angle of impingement, temperature of environment, and subcritical crack growth on erosion rate and related strength degradation for Al_2O_3, SiC, and Si_3N_4. Biaxial strength characterizations of as-prepared and eroded samples.

MICHIGAN STATE UNIVERSITY

382. STUDIES ON AGE HARDENING IN SPINODALLY MODULATED ALLOYS - EXPERIMENTAL AND THEORETICAL

K. N. Subramanian - Dept. of Metallurgy, Mechanics, and Materials Science
Phone: (513)-353-5197, (513)-355-5147

$ 60,653 01-2

Structure-property relationship and age-hardening of the spinodal alloy system Cu-10%Ni-6%Sn. Single crystal studies of mechanical properties of both one dimensionally and three dimensionally modulated alloys. Dislocation mobility studies by in-situ TEM (with deformation stage) experiments. Application and development of elasticity and hardening theories to various multi-phase morphologies associated with the spinodal decomposition reaction. Computer analysis of the energetics of dislocation double-kink formation and for thermally activated dislocation motion. Experiments and theory concerning temperature and strain-rate dependent mechanical behavior.

MICHIGAN TECHNOLOGICAL UNIVERSITY

383. ENVIRONMENT-INDUCED EMBRITTLEMENT: EFFECTS OF IMPURITY SEGREGATION AND STATE OF STRESS

L. A. Heldt - Dept. of Metallurgical Engineering
Phone: (906)-487-2630
D. A. Koss - Dept. of Metallurgical Engineering
Phone: (906)-487-2170

$118,000 (17 months) 01-2

Hydrogen embrittlement and stress corrosion cracking behavior and the influence of grain boundaries and multiaxial stresses on these phenomena. Effect of hydrogen on tensile properties and local plastic strain in bicrystals of Ni. Influence of grain boundary motion on interfacial diffusivity. Multiaxial fracture criteria for hydrogen embrittlement and stress corrosion cracking as influenced by microstructure. Influence of multiaxial loading on stress corrosion cracking in brass, and hydrogen embrittlement in Ni, Zr, and Zr alloy.

UNIVERSITY OF MICHIGAN

384. SURFACE-PLASMON EXPLORATION OF MULTILAYER PHYSISORBED AND CHEMISORBED FILMS ON METAL SUBSTRATES

M. Bretz - Dept. of Physics
Phone: (313)-764-4494

$ 50,000 02-2

Measurements of dielectric properties of adsorbed films by laser excitation of surface plasmons. Technique permits study of phase transitions in monolayer to multilayer films, following layer-by-layer evolution of films from two to three dimensions, detecting orientational effects of non-spherical adsorbed molecules, and study of a variety of other surface phenomena.

385. EFFECT OF CRYSTALLIZATION OF GRAIN BOUNDARY PHASE ON THE HIGH TEMPERATURE STRENGTH OF SILICON NITRIDE CERAMICS

T. Y. Tien - Dept. of Materials and Metallurgical Engineering
Phone: (313)-764-9449

$ 79,000 01-1

Study of role and mechanism of nucleating agents on the crystallization of the Si_2N_2O containing grain boundary phases which are formed during the processing of Si_3N_4 (containing Y_2O_3 and Al_2O_3) and SIALON ceramics. Microstructure and phase identification in sintered and hot pressed specimens. X-ray diffraction, scanning transmission electron microscopy, electron energy loss spectroscopy, fractography analysis.

386. A SYSTEMATIC APPROACH TO INTERGRANULAR CRACKING MECHANISMS IN AUSTENITIC ALLOYS THROUGH GRAIN BOUNDARY CONTROL

G. S. Was - Dept. of Nuclear Engineering
Phone: (313)-763-4675

$100,000 (15 months) 01-2

Experimental investigation of intergranular stress corrosion cracking of Ni-base austenitic alloys in aqueous solutions, using Huey, Streicher, and constant extension rate tests; grain boundary composition (Cr and P level) and carbide distribution monitored with TEM and AES.

UNIVERSITY OF MINNESOTA

387. A MICROSTRUCTURAL APPROACH TO FATIGUE CRACK PROCESSES IN POLYCRYSTALLINE BCC MATERIALS

W. W. Gerberich - Dept. of Chemical Engineering and Materials Science
Phone: (612)-373-4829

$ 83,900 01-2

Investigation of deformation-fracture-microstructure interrelationships in fatigue of Fe, Fe-Si alloys, high strength low alloy steels, and Ti-30 Mo; modelling of mechanical properties--strain rate sensitivity, flow stress and its temperature dependence, and monotonic vs cyclic loading effects; influence of microstructural features such as grain size and slip characteristics; analysis of cyclic strain hardening exponent and ductile-brittle transition temperature; modelling in terms of dislocation dynamics and fracture toughness parameters; crack closure and its effect on fatigue threshold; H_2 effects on the above; techniques used: electron channeling, SEM, TEM.

388. EXPERIMENTAL STUDY OF THE THERMODYNAMICS OF THIN FILMS AND SURFACES

A. M. Goldman - School of Physics
Phone: (612)-373-5480
E. D. Dahlberg - School of Physics
Phone: (612)-373-3358

$ 70,000 02-2

Development of a calorimeter especially suited to the study of the heat capacities of extremely thin films. Integrated circuit techniques which have been used to fabricate single-crystal silicon membrane Josephson tunneling junctions will be applied. If successful, the calorimeter will be used to study inversion layers of Si-MOS structures and phase transitions of monolayers on silicon single crystals. Auger spectroscopy and LEED used to study structure of adsorbent and adsorbate.

UNIVERSITY OF MINNESOTA (continued)

389. CORROSION RESEARCH CENTER

R. Oriani - Dept. of Chemical Engineering and Materials Science
Phone: (612)-373-4864

$945,000 01-1

Research and technology transfer in corrosion; multidisciplinary approach to corrosion research; theory of the double layer and electron transfer at solid-fluid interfaces; plasma-sprayed coatings; laser surface modification; adhesion of polymeric coatings; plasma-processed polymer coatings; healing processes at polymer-polymer interfaces; stress corrosion resistance of polymers in the presence of plasticizers; infrared laser-induced reactions at solid-gas interfaces; reduction and cyclic fatigue of oxide films; measurements of the oxidation state of GaAs, Fe, and Zn alloys with Auger electron and X-ray spectroscopies and other electrochemical methods; high temperature oxidation of Fe-Cr-Al alloys in gases with a range of O:S activities; hot corrosion of oxide scales in molten sulfates.

UNIVERSITY OF MISSOURI/COLUMBIA

390. DEVELOPMENT AND CHARACTERIZATION OF HIGH TEMPERATURE ELECTRICALLY CONDUCTING OXIDES

H. E. Anderson - Dept. of Ceramic Engineering
Phone: (314)-341-4886, 4401

$112,000 01-3

Interrelationship of electrical conductivity, oxidation-reduction kinetics, defect structure, and composition for n type transition metal oxides TiO_2, $SrTiO_3$, and $BaTiO_3$ and p type transition metal oxides Cr_2O_3, NiO, $LaCrO_3$, and $YCrO_3$. Experimental aspects include specimen preparation, thermogravimetric measurements, X-ray diffraction, transmission electron microscopy, and magnetic susceptibility, Hall, conductivity, and Seebeck measurements.

UNIVERSITY OF MISSOURI/COLUMBIA (continued)

391. INELASTIC SCATTERING IN CONDENSED MATTER WITH HIGH INTENSITY MÖSSBAUER RADIATION

W. B. Yelon - Dept. of Physics
Phone: (314)-882-4211
G. Schupp - Dept. of Physics
Phone: (314)-882-4211
J. G. Mullen - Dept. of Physics, Purdue University
Phone: (317)-494-3031

$175,000 (19 months) 02-2

Using the unique source of Tungsten-183 46.5 keV Mössbauer radiation at the University of Missouri, a variety of condensed matter science experiments will be undertaken. The intensity of the available radiation is about one thousand times more intense than that used in most Mössbauer Spectroscopy, and a special MIcroscopic Conversion Electron (MICE) detector will be developed and employed in this program. The initial experiments will separate the elastic and inelastic scattering at Bragg reflections, determine the quasielastic linewidths observed in critical phenomena and studies of very low energy Landau excitations.

UNIVERSITY OF MISSOURI/KANSAS CITY

392. ELECTRONIC PROPERTIES OF AMORPHOUS SILICON DIOXIDE AND METALLIC IONS IN SILICATE GLASSES

W-Y. Ching - Dept. of Physics
Phone: (816)-276-1604

$ 40,000 01-1

Theoretical study of the electronic properties of crystalline SiO_2, Si_3N_4, silicon oxynitrides, alkali silicates, amorphous SiO_2, and silicate glasses containing impurities such as hydrogen, hydroxl, alkali, and transition metal ions by the OLCAO method. Results concern electron density of states, energy band gaps, chemical bonding, charge transfer and charge density distribution, local density of states, optical absorptions, etc. Nature and location of impurity states of various ions in the silicate glass network, and impurity-host interactions. Comparison of calculated local density of states with UPS and XPS measurements underway at Argonne National Laboratory. Development of a direct-space self-consistent field method for the electronic structure calculation within the LCAO framework.

NATIONAL BUREAU OF STANDARDS

393. INTERAGENCY PROGRAM FOR SUPPORT OF CRITICAL DATA COMPILATIONS

D. R. Lide - Office of Standard Reference Data
Phone: (301)-921-2467

$200,000

Support for the critical evaluation of data in the physical sciences and for the preparation of compilations of standard reference data is being provided through a collaborative program involving the National Bureau of Standards, National Science Foundation, Office of Naval Research, and the Department of Energy. Thermodynamic and phase equilibria data evaluation and compilation represent the principal thrust of this program.

UNIVERSITY OF NEVADA

394. PHOTOPHYSICAL STUDIES OF TRIPLET EXCITON PROCESSES IN PURE POLYMER FILMS

R. D. Burkhart - Dept. of Chemistry
Phone: (702)-784-6041

$ 78,347 03-1

Evaluate photophysical rate constants relevant to solid films of poly (N-vinylcarbazole) and related to photon collection and energy transmission.

NEW MEXICO INSTITUTE OF MINING AND TECHNOLOGY

395. MICROSTRUCTURAL AND MECHANICAL PROPERTY STUDY OF SOLAR ENERGY COLLECTORS

O. T. Inal - Dept. of Metallurgical and Materials Engineering
Phone: (505)-835-5229, 5519

$ 95,000 (24 months) 01-1

Effect of plating geometry, bath compositions and current densities on the surface structure of electroplated black Cr_2O_3 and anodic oxidation of leaf Zn, Zn electroplated steel, and hot-dip galvanized steel. TEM, FIM, nucleation, solar absorption, thermal cycle, mechanical adhesion studies, ZnO and Al_2O_3 film coatings, copper oxide and black nickel selective surfaces, and mathematical optimization of selective solar surfaces.

UNIVERSITY OF NEW MEXICO

396. RADIATION EFFECTS AND ANNEALING KINETICS IN CRYSTALLINE SILICATES, PHOSPHATES, AND COMPLEX Nb-Ta-Ti OXIDES

R. C. Ewing - Geology Dept.
Phone: (505)-277-2030

$ 95,000 01-1

Comparative study of the properties of selected metamict minerals and synthetic irradiated phases of similar composition. In order to correlate radiation effects in synthetic phases (e.g., fission track formation and fading) with the process of metamictization, the following properties of metamict minerals will be examined: (a) refractive index birefringence and density (b) microstructure, (c) annealing kinetics, and (d) leach behavior. One of the major effects of this part of the study will be the determination of the structure of the metamict state by the use of electron microscopy and extended X-ray absorption fine structure spectroscopy. Annealing and recrystallization kinetics of the metamict and partially metamict phases.

CITY UNIVERSITY OF NEW YORK/BROOKLYN COLLEGE

397. OPTICAL AND ELECTROCHEMICAL INVESTIGATION OF RUTHENIUM AND IRIDIUM AND THEIR OXIDES IN RELATION TO THEIR ELECTROCATALYTIC ACTIVITY

F. H. Pollak - Dept. of Physics
Phone: (212)-780-5356

$164,000 (18 months) 03-3

Studies of factors affecting behavior of single-crystal Ru and Ir oxides as electrocatalysts for the O_2 evolution reaction. Determination of electronic energy levels and density of states from optical and u.v. photoemission, Raman and infrared spectroscopy. In situ electrochemical and combined electrochemical-optical measurements.

CITY UNIVERSITY OF NEW YORK/CITY COLLEGE

398. ELECTRONIC AND OPTICAL PROPERTIES OF DISORDERED SYSTEMS

M. Lax - Dept. of Physics
Phone: (212)-690-6864

$ 85,000 02-3

An extensive theoretical study of transport and optical properties of disordered media such as amorphous materials, doped semiconductors, quasi-one dimensional conductors, interfaces, etc.

CITY UNIVERSITY OF NEW YORK/CITY COLLEGE (continued)

399. STUDY OF FORMATION OF SURFACE FILMS: CRITICAL CONDITIONS FOR GROWTH

F. W. Smith - Dept. of Physics
Phone: (212)-690-6963

$ 42,529 01-5

Experimental studies of the critical conditions for growth of surface films in a UHV reaction system with pressure of the gaseous reactants and substrate temperature as the primary variables. Principal systems under investigation consist of (1) silicon nitride and oxynitride films formed via reaction of NO with Si(111) and Si(100), (2) silicon carbide formed via the interaction of C_2F_4 or $C_2H_2F_2$ with Si(111) and Si(100) and (3) silicon carbide formed via the CH_4 + Si reaction. Analytical techniques include scanning electron microscopy, Auger electron spectroscopy, X-ray photoemission spectroscopy at the BNL-NSLS.

POLYTECHNIC INSTITUTE OF NEW YORK

400. PHOTOEMISSION STUDIES OF f-ELECTRON SYSTEMS: MANY BODY EFFECTS

R. D. Parks - Dept. of Physics
Phone: (212)-643-2070

$ 75,000 02-2

Photoemission studies of rare earth systems, particularly intermetallic compounds, aimed at understanding electronic phenomena underlying the 4f instabilities in mixed valent and Kondo lattice systems. Synchrotron radiation is a major experimental tool in these studies.

STATE UNIVERSITY OF NEW YORK/STONY BROOK

401. CONSTRUCTION AND MAINTENANCE OF SUNY FACILITIES AT THE NATIONAL SYNCHROTRON LIGHT SOURCE (Several Institutions Involved)

J. Bigeleisen - Dept. of Chemistry
Phone: (516)-246-7945

$300,000 02-2

An X-ray beam line is being built and instrumented at the National Synchrotron Light Source (NSLS) under the auspices of this Participating Research Team (PRT). This PRT represents campuses at Albany, Buffalo, Stony Brook, Cortland, and Alfred. This line will include facilities for high resolution crystallography, surface physics, small angle scattering, and EXAFS.

STATE UNIVERSITY OF NEW YORK/STONY BROOK (continued)

402. SYNCHROTRON TOPOGRAPHIC PROJECT PARTICIPATING RESEARCH TEAM (Several Institutions Involved)

J. C. Bilello - Dept. of Materials Science and Engineering
Phone: (516)-246-5983

$460,000 01-1

Conclusion of initial phase design and construction of beam-line X-19 at the National Synchrotron Light Source so that a basic work station furnished with an operational White Beam Camera (WBC) and a Multiple Crystal Camera (MCC) for monochromatic topography. This Synchrotron Topography Project for the NSLS facility beam-line will develop a research effort on a range of scientific problems where Synchrotron Topography can make unique contributions. Absorption edge contour and synchrotron x-ray fractography to characterize individual dislocations and local strain fields. Scientific work encompasses characterization of Si chips and metal-silicide thin films, local strain studies in CdS after pressure quenching, studies on fracture in tungsten bi-crystals and of the role of grain boundaries in high temperature failure, thermal decomposition studies in inorganic crystals, investigations of fundamental fracture mechanisms of semi-brittle materials, and studies of the interaction of acoustic waves with microstructure and defects in structural and electronic materials.

403. SURFACE STUDIES: A PROPOSAL FOR A PARTICIPATING RESEARCH TEAM AT NSLS

F. Jona - Dept. of Materials Science and Engineering
Phone: (516)-246-7649, 6759

$242,236 (20 months) 02-2

Development of a versatile, high-vacuum experimental chamber for surface research with the VUV ring at NSLS: chamber will include LEED, Auger, and photoemission facilities. Studies of atomic structure of solid surfaces: Al, Fe, and Ti, both clean and with O, S, Cl, and CO adsorbates; SEXAFS. Chemisorption, physisorption and hydrogen uptake: H uptake by Nb; O on Ni and Nb; Pd on Nb and Ta. Electronic properties of solids: lifetimes of excited states in metals and insulators; effects of bulk phase transitions on surface structure; surface and bulk properties of FeTi.

STATE UNIVERSITY OF NEW YORK/STONY BROOK (continued)

404. CHEMISORPTION THEORY: ADSORPTION ON COPPER-NICKEL ALLOYS AND TITANIUM SURFACE EMBRITTLEMENT

J. L. Whitten - Dept. of Chemistry
Phone: (516)-246-6068, 5050

$ 90,000 03-3

An embedding theory for treating chemisorption on metals extended and applied to systems involving Ti, Cu, Ni and Cu/Ni alloy and H_2, H, Co, C, and coabsorbed H and C adsorbates. Emphasis on the energetics of adsorption as a function of surface site and composition to determine the reactivity of adsorbed species.

NORTH CAROLINA AGRICULTURAL AND TECHNICAL UNIVERSITY

405. EFFECT OF FATIGUE AND THERMAL LOADS ON SILICON CARBIDE REINFORCED GLASS MATRIX COMPOSITES

V. S. Avva - Dept. of Mechanical Engineering
Phone: (919)-379-7620
J. Sankar - Dept. of Mechanical Engineering
Phone: (919)-379-7620

$ 50,000 01-5

Structural characterization of SiC/glass matrix fibers before, during, and after tension and thermal fatigue testing from room temperature to 650°C at a stress amplitude ratio of 0.1 and a frequency of 10Hz. Radiographic examination for delaminations, debonding, fiber breakage, etc. Optical and scanning electron microscopy microstructural characterization.

NORTH CAROLINA STATE UNIVERSITY

406. DEVELOPMENT OF AN X-RAY BEAM LINE AT THE NSLS FOR STUDIES IN MATERIAL SCIENCE USING X-RAY ABSORPTION SPECTROSCOPY (Several Institutions Involved)

D. E. Sayers - Dept. of Physics
Phone: (919)-737-2512

$275,000 02-2

Development of an advanced X-ray absorption fine structure (EXAFS) beam line at NSLS for a Participating Research Team (PRT) with members from North Carolina State University, University of Connecticut, University of Washington, University of Delaware, Brookhaven National Laboratory, United Technologies and General Electric. Facility will cover the energy range from 1-20 KeV and include provisions for transmission EXAFS, fluorescence EXAFS, surface EXAFS and X-ray absorption studies. Materials science research to be addressed includes areas of metallurgy, corrosion, amorphous materials, catalysis, surface science, electrochemistry and magnetic properties.

407. THE EFFECT OF MICROSTRUCTURE OF SOLID-PARTICLE EROSION IN MULTIPHASE MATERIALS

R. O. Scattergood - Dept. of Materials Engineering
Phone: (919)-737-2377
H. Conrad - Dept. of Materials Engineering
Phone: (919)-737-2377

$ 90,000 (13 months) 01-5

Correlation of erosion rates in multiphase alloys with constituent phase properties, morphology, and distribution; systems to be studied include ductile-brittle mixtures (e.g., Al-Si, Co-Al, Ni-Al_2O_3) and brittle materials (e.g., oxides); modelling of erosion to derive constitutive laws; computer simulation.

NORTHEASTERN UNIVERSITY

408. DYNAMICAL FRICTION IN CONDENSED MATTER

J. B. Sokoloff - Dept. of Physics
Phone: (617)-437-2931
C. H. Perry - Dept. of Physics
Phone: (617)-437-2913

$ 81,000 02-3

Joint theoretical-experimental studies of a variety of systems reflecting motion of one set of species (ions, defects, layers) relative to another set of species (channels, lattices, layers). The rate of energy dissipation, its frequency, temperature and pressure dependence will be calculated as well as electronic contributions to the damping. Experimental studies of Y_2O_3 - ZrO_2, hollandite perovskite, intercalated graphite and dichalcogenides will be related to the theoretical models, including a predicted electric field effect.

NORTHWESTERN UNIVERSITY

409. DEFECT CLUSTERS AND ELECTRICAL PROPERTIES IN TRANSITION METAL MONOXIDES

J. B. Cohen - Dept. of Materials Science and Engineering
Phone: (312)-492-3570
D. E. Ellis - Dept. of Physics and Astronomy
Phone: (312)-492-3665
T. O. Mason - Dept. of Materials Science and Engineering
Phone: (312)-492-3198

$112,240 (10 months) 01-1

Measurements of defect structure and electrical properties and quantum theoretical calculations for multicomponent transition metal oxides. Electrical measurements and analysis based on Arrhenius plots of conductivity at constant Seebeck coefficient for MnO and NiO. Valence studies via X-ray absorption edge, TEM critical voltage technique, and photoelectron spectroscopy. Defect interaction studies in MnO and CoO via X-ray (synchrotron at the BNL NSLS) and pulsed neutron scattering (at the ANL IPNS). Preliminary electrical and structural studies of ScO and CrO. Self-consistent-field local density theory calculations for the electronic structure associated with isolated vacancies and defect clusters. Use of an energy band code based on the Linearized Muffin Tin Scheme to calculate and compare band structures, Fermi surfaces, and transport properties with experimental studies.

NORTHWESTERN UNIVERSITY (continued)

410. ULTRA-LOW-TEMPERATURE NEUTRON DIFFRACTION

W. P. Halperin - Dept. of Physics and Astronomy
Phone: (312)-492-3686, 3644
J. B. Ketterson - Dept. of Physics and Astronomy
Phone: (312)-492-5468, 3644

$110,000 (24 months) 02-1

Using an ultralow temperature neutron diffraction facility at Argonne National Laboratory, nuclear magnetic ordering phenomena will be investigated. The primary effort will be a determination of the nature of the nuclear ordering in solid helium-3, a result of fundamental importance. The program will also investigate the ordering of nuclear spins in metals such as $PrCu_6$.

411. EFFECT ON POINT DEFECTS ON MECHANICAL PROPERTIES OF METALS

M. Meshii - Dept. of Materials Science
Phone: (312)-492-3213

\$ 87,000 01-2

Experimental and analytical investigation of low temperature flow behavior of Nb; influence of crystallographic orientation and interstitial atoms on deformation by primary vs anomalous slip; H_2 effects on dislocation motion, low temperature on hardening and softening, as well as on fracture of Fe by intergranular quasi-cleavage or microvoid coalescence; trapping of H_2 and S impurities.

412. AN INVESTIGATION OF MICROSTRUCTURAL CHANGES IN FERRITIC STAINLESS STEELS CAUSED BY HIGH TEMPERATURE DEFORMATION

J. R. Weertman - Dept. of Materials Science and Engineering
Phone: (312)-492-5353

\$ 63,275 01-2

Investigation of deformation, failure, and microstructural stability during creep and creep fatigue in low alloy ferritic steels; TEM and SANS characterization of strain and thermal induced microstructural modifications, e.g., carbide precipitation, cavity formation; influence of prestrain on residual stress and hydrogen attack.

NORTHWESTERN UNIVERSITY (continued)

413. INVESTIGATION OF DEEP LEVEL DEFECTS IN EPITAXIAL SEMICONDUCTING ZINC SULPHO-SELENIDE

B. W. Wessels - Dept. of Materials Science and Engineering
Phone: (312)-492-3219

$ 64,395 01-3

Investigation of fundamental point defect formation mechanisms in the wide bandgap semiconductor ZnSSe. Identification of deep level defects in deliberately doped and MeV electron irradiated material and exploration of their role in electrical compensation. Thermal stability of defects. Experimental techniques include optical and electrical deep level transient spectroscopy, Hall measurements, photocapacitance, and spectrally resolved photocurrent measurements.

414. BASIC RESEARCH ON CERAMIC MATERIALS FOR ENERGY STORAGE AND CONVERSION SYSTEMS

D. H. Whitmore - Dept. of Materials Science and Engineering
Phone: (312)-492-3533

$ 71,500 01-1

Investigation of factors affecting electronic and mass transport behavior in solid electrolyte and electrode materials; study of the effect of a dispersed second (non-soluble) phase on ionic transport in solid electrolytes; synthesis and characterization of new materials which may have application as solid electrodes or electrolytes in energy storage or conversion; and optimization of the factors affecting the fabrication and ion transport properties of dense polycrystalline specimens of new solid electrolyte and electrode materials. Techniques employed include ac conductivity, dc polarization measurements, tracer diffusion, dielectric loss, ion thermal current measurements, Raman spectroscopy, NMR line-narrowing and pulsed field gradient experiments, chemical preparation and crystal growth of selected electrolyte materials. Materials under investigation include mixed ammonium and hydrogen beta"-aluminas, their deuterated counterparts, and analogous gallates; Li_2O-LiCl-B_2O_3 and Li_2O-LiF-B_2O_3 glasses; and LiI-silica composites.

UNIVERSITY OF NOTRE DAME

415. MICROSTRUCTURAL EFFECTS IN ABRASIVE WEAR

T. H. Kosel - Dept. of Metallurgical Engineering and Materials Science
Phone: (219)-239-5642

$ 90,000 01-5

Assessment of mechanisms controlling abrasive wear in multiphase alloys, including cast iron; influence of abrasive hardness and angularity; role of wear debris; in-situ SEM scratch tests; change in near-surface microstructure under abrasive wear conditions.

OHIO STATE UNIVERSITY

416. INVESTIGATIONS OF ULTRASONIC WAVE INTERACTIONS AT BOUNDARIES SEPARATING ANISOTROPIC MEDIA

L. Adler - Dept. of Welding Engineering
Phone: (614)-422-1974

$ 90,000 01-5

Research into the interaction of ultrasonic waves with boundaries separating anisotropic materials. Single crystals and bicrystals of nickel are prepared for ultrasonic measurements. Measurements are made of the partitioning of wave energy at an anisotropic-anisotropic boundary and analytical treatment of wave propagation at anisotropic boundaries is included.

417. INFLUENCE OF NITROGEN ON THE SENSITIZATION, CORROSION, MECHANICAL AND MICROSTRUCTURAL PROPERTIES OF AUSTENITIC STAINLESS STEELS

W. A. T. Clark - Dept. of Metallurgical Engineering
Phone: (614)-422-2538
D. D. Macdonald - Dept. of Metallurgical Engineering
Phone: (614)-422-6255

$ 85,470 (15 months) 01-1

Evaluation of corrosion and stress corrosion cracking of austenitic stainless steel with various C and N contents; TEM characterization of grain boundary structure as well as carbide and nitride morphologies and distribution; measurement of electrochemical parameters in static and flowing aqueous solutions containing chloride and sulphate ions.

OHIO STATE UNIVERSITY (continued)

418. FUNDAMENTAL STUDIES OF HIGH TEMPERATURE CORROSION REACTIONS

R. A. Rapp - Dept. of Metallurgical Engineering
Phone: (614)-422-6178

\$ 88,000	01-1

In-situ SEM study of oxidation of metals, Fe, Ni, Cu and Cr; effect of H_2 on oxide morphology; influence of surface treatment on oxidation of Cr; pore development at metal-scale interface; oxide morphologies, e.g., pits and ledges in Fe_2O_3 and whiskers in NiO.

419. HYDROGEN ATTACK OF PRESSURE VESSEL STEELS

P. G. Shewmon - Dept. of Metallurgical Engineering
Phone: (614)-422-2491

\$ 66,107	01-2

The mechanisms which determine the rate of hydrogen attack of pressure vessel steel are studied through a combination of growth kinetic measurements (dilalometry) and careful metallorgraphy. The origin of bubble nuclei is given particular emphasis. In this connection the relative rates of attack in thick section welds and the role of fine weld porosity is given emphasis. The role of matrix creep restraint in limiting hydrogen attack kinetics is studied.

OREGON STATE UNIVERSITY

420. INVESTIGATION OF THE ELECTRICAL AND OPTICAL PROPERTIES OF ORGANOMETALLIC VAPOR PHASE EPITAXIAL $Ga_{1-x}Al_xAs$ AND $Ga_{1-x}Al_xAs/GaAs$ INTERFACES IN SOLAR CELLS

P. K. Bhattacharya - Dept. of Electrical and Computer Engineering
Phone: (503)-754-3617

\$ 69,098	01-3

Electrical and optical characterization of undoped and intentionally doped $Ga_{1-x}Al_xAs$ layers and $Ga_{1-x}Al_xAs/GaAs$ interfaces grown by organometallic vapor phase epitaxial (OMVPE) growth. Measurements extend over the entire mixed alloy composition range of the ternary alloy with particular emphasis on the indirect bandgap region ($x \geq 0.43$) being used for concentrator heterostructure solar cells. Electrical characterization includes detailed study of deep trapping centers in bulk layers and interface regions and transport properties in these regions as a function of alloy composition and temperature. Optical studies include characteristics of the deep states and luminescence measurements. Measurement techniques are Deep Level Transient Spectroscopy, Double Source Differentiated Photocapacitance, capitance-voltage, Hall-effect, velocity-field, and photoluminescence.

PENNSYLVANIA STATE UNIVERSITY

421. HEAT TRANSFER, FLUID FLOW AND ELEMENT VAPORIZATION IN LASER WELDING

T. DebRoy - Dept. of Materials Science and Engineering
Phone: (814)-865-1974

$ 51,400 01-5

Modelling of solute loss during laser welding of steels based on solution thermodynamics and kinetics data; calculation of local cooling rate and temperature profile, weld pool velocity and propensity for grain growth; correlative experimental determination of weld microstructure and chemistry; measurement of hardness across the weld.

422. CRYSTAL CHEMISTRY OF PORTLAND CEMENT HYDRATES AS RADIOACTIVE WASTE HOSTS

M. W. Grutzeck - Materials Research Laboratory
Phone: (814)-865-3539

$ 50,003 01-1

Detailed study of the crystal chemistry of various hydrated cement phases. Identification of possible crystal chemical substitutions for radioactive waste ions in the crystal structures of the various cement hydrates. Evaluation of the stabilities of substituted cement hydrates. Assemblage of a library of crystal chemical data to be used to optimize cement compositions for use in radioactive waste management.

423. STRUCTURAL PROPERTIES OF AMORPHOUS METALS BY RAMAN SCATTERING

J. S. Lannin - Dept. of Physics
Phone: (814)-865-9231

$ 78,892 01-1

This study involves the preparation of thin films of amorphous metal alloys by sputtering methods. The optical constants of these films are employed to fabricate trilayer structures for the study of Raman scattering. The materials to be considered initially are iron-boron and iron-phosphorus alloys. The goal of the study is to obtain information on the structure, bonding and thermal stability as a function of temperature, alloy concentration and sputter deposition conditions. The work involves the study of both amorphous and crystalline metal alloys using trilayer Raman scattering.

PENNSYLVANIA STATE UNIVERSITY (continued)

424. MECHANISMS OF WEAR IN SINGLE AND TWO PHASE MATERIALS

N. H. Macmillan - Materials Research Laboratory
Phone: (814)-863-0180

$ 60,900 (19 months) 01-5

Experimental investigation of two body wear in metals (Al, Cu) and ceramics (Al_2O_3, MgO); effect of contact zone, strain rate and deformation/fracture characteristics of materials.

425. LASER PROCESSING OF CERAMICS

G. L. Messing - Dept. of Materials Science and Engineering
Phone: (814)-865-2262

$ 97,000 (18 months) 01-5

Studies of single component, multicomponent, and decomposition-reaction laser-particle interactions in fine-particle ceramics. Use of a 10.6 micron CO_2 laser to effect calcination without aggregation, morphological modification of particles, and comminution. Thermodynamic and kinetic assessment of effects of rapid heating on processes in fine-particle ceramics, with concerns for potential melting, metamictization, vaporization, and microcracking phenomena. Initial studies will be on Al_2O_3 and MgO particles and their precursors.

426. HYDROGEN ABSORPTION IN METALS: A FIELD ION MICROSCOPY STUDY

H. W. Pickering - Dept. of Materials Sciences and Engineering
Phone: (814)-863-2640

$ 54,000 01-1

Field ion microscopy study of H_2 trapping and absorption in Fe; surface and grain boundary segregation of P and Ti in Ni and H in Fe; quantitative measure of the concentration gradients away from boundaries; cosegregation and clustering of impurities; relationship of above to embrittlement of alloys.

PENNSYLVANIA STATE UNIVERSITY (continued)

427. GRAIN BOUNDARY DIFFUSION AND GRAIN BOUNDARY CHEMISTRY OF CR-DOPED MAGNESIUM OXIDE

V. S. Stubican - Dept. of Materials Science
Phone: (814)-865-9921

$ 52,500 01-3

Aliovalent impurity diffusion in ionic materials, specifically Cr in MgO; binding energy between impurities and vacancies; grain boundary diffusion, including diffusion parallel and perpendicular to tilt boundaries; surface diffusion; techniques used--autoradiography, electron microprobe, ion beam spectrochemical analysis.

428. STUDY OF FIELD ADSORPTION USING IMAGING ATOM-PROBE FIELD ION MICROSCOPY

T. T. Tsong - Dept. of Physics
Phone: (814)-865-2813

$ 60,000 02-2

To study in atomic detail the field adsorption of noble gases and classical molecular gases using the imaging atom probe field ion microscope. Measure the adsorption energy as a function of field on catalytically active group VIII metal surfaces. Mechanism of formation of metal-noble gas complex ions. Photon and electron stimulated field desorption.

429. STRUCTURE OF GLASSES CONTAINING TRANSITION METAL IONS

W. B. White - Materials Research Laboratory
Phone: (814)-865-1152

$110,000 01-1

Structure and behavior of (1) insulator glasses: silicates, borates, germanates, and phosphates, and (2) modified insulator glasses containing transition metal ions. Leaching and dissolution behavior of glasses. Host glass structure is determined by infrared and Raman spectroscopy. Observed vibrational spectra are related to structural units that make up the glass by means of normal coordinate and other theoretical calculations. Characterization of nearest neighbor environments of transitional metal ions in glasses are carried out by optical absorption spectra, luminescence spectra, and vibrational bands.

UNIVERSITY OF PENNSYLVANIA

430. HIGH CONDUCTIVITY PROTON SOLID ELECTROLYTES

G. C. Farrington - Dept. of Materials Science and Engineering
Phone: (215)-898-6642

$ 94,178 03-1

Preparation and characterization of a series of solid state protonic conductors, for use in the temperature range of 100-400°C. Determination of conductivities of NH_4^+-H^+-β aluminas, and studies of the influence of the stabilizing cation. Studies on single crystals of deuteronium beta and beta" alumina including refinements of atomic positions, band lengths, etc. NMR studies will be employed to explore microscopic processes of diffusion.

431. MECHANISMS OF DAMAGE ACCUMULATION IN TIME DEPENDENT CYCLIC DEFORMATION

C. Laird - Dept. of Metallurgy and Materials Science
Phone: (215)-898-6664

$ 63,500 01-2

Identification of microstructural changes resulting from creep and fatigue deformation of metals, initially Cu and low alloy steels; correlation of substructure development with strain hardening and softening during prior monotonic, interrupted or reversed stress cycles; strain burst and relationship to substructure instability; effect of carbide distribution in bainitic steels on strength and transition from trans- to intergranular failure mode; extension of Coffin-Manson low cycle fatigue relation to cyclic creep.

432. INTRINSIC SURFACE PHONONS ON RECONSTRUCTED SEMICONDUCTOR SURFACES

E. J. Mele - Physics Dept.
Phone: (215)-898-3135

$ 78,715 02-3

Theoretical study of the lattice dynamics of reconstructed semiconductor surfaces. Relation between localized surface electronic properties and surface structural and vibrational properties. Computational scheme combines a short range elastic Hamiltonian with a static electronic polarizability extracted from a tight binding representation of the valence electronic bands.

UNIVERSITY OF PENNSYLVANIA (continued)

433. ATOMISTIC STUDIES OF GRAIN BOUNDARIES WITH SEGREGATED IMPURITIES

V. Vitek - Dept. of Metallurgy and Materials Science
Phone: (215)-898-7883

$ 75,000 01-1

Atomistic-based computer simulation of grain boundary structure in dilute and concentrated binary metal alloys, initially Au-Ag, Cu-Ag, and Cu-Bi; development of semi-empirical interatomic potentials incorporating charge transfer and atomic volume and fitted to satisfy lattice parameter and cohesive energy requirements; influence of degree of segregation and boundary periodicity; computation of stress fields around impurities at grain boundaries, and effect of this on co-segregation and H_2 trapping at boundary; structural transitions at boundaries and influence on defect absorption or emission.

434. ELECTROCHEMICAL INVESTIGATIONS OF NOVEL ELECTRODE MATERIALS

W. L. Worrell - Dept. of Materials Science and Engineering
Phone: (215)-898-8592

$ 60,000 03-2

Intercalation of Li, Na and Ca into TiS_2 to form $Li_yNa_yTiS_2$ and $Li_yCa_yTiS_2$, resulting in increased electrical capacity of cathode materials for advanced batteries. Electrochemical studies of electrode performance, and X-ray structural determination of intercalated compounds. Measurement of diffusion coefficient of Li ions; studies of effect of ionic size and charge on stability of intercalant in the TiS_2 lattice. Structural and phase analysis studies will be completed and an isothermal section of the Li-Na-TiS_2 pseudoternary phase diagram will be constructed. Effect of transition metals on Li-Li interaction energy in $Ti_{1-y}Ta_yS_2$ and $Ti_{1-y}Zr_yS_2$.

UNIVERSITY OF PITTSBURGH

435. HIGH TEMPERATURE CORROSION OF CERAMICS

F. S. Pettit - Dept. of Metallurgical and Materials Engineering
Phone: (412)-624-5300
J. R. Blachere - Dept. of Metallurgical and Materials Engineering
Phone: (412)-624-5296

$ 65,000 01-3

Thermodynamic and kinetic analyses of gaseous and molten salt corrosion of oxides (SiO_2, Al_2O_3, Cr_2O_3, and ZrO_3) in oxidizing, sulfidizing, and reducing environments; thermogravimetric measurement of corrosion kinetics.

PRINCETON UNIVERSITY

436. STUDIES OF THE DYNAMICS OF MOLECULAR ORIENTATION AND RELAXATION IN POLYMERS BY MEANS OF A MODULATED INFRARED LINEAR DICHROISM TECHNIQUE

J. T. Koberstein - Dept. of Chemical Engineering
Phone: (609)-452-5721
R. K. Prud'homme - Dept. of Chemical Engineering
Phone: (609)-452-4577

$ 72,724 03-1

Examine the fundamental relationship between chain conformational changes and resultant macroscopic material responses during deformation. Coupling of rheological and rheo-optical measurements during weld characterized deformation in order to follow the details of molecular orientation and conformational changes.

PURDUE UNIVERSITY

437. NOVEL POLYMERIC Li^+ AND Cd^{2+} FAST ION CONDUCTING MATERIALS; LiI-IODIDE IONENE POLYMERS AND CdI_2-$Cd(PO_3)_2$/$Cd(PS_3)_2$ GLASSES

C. A. Angell - Dept. of Chemistry
Phone: (317)-494-5256
E. I. Cooper - Dept. of Chemistry
Phone: (317)-494-5256

$ 52,201 01-1

Preparation of plastic fast ion conductors via the formation of a "molten salt" system by dissolution of lithium salts, especially LiI, in iodides of quaternary nitrogen polymeric cations (ionenes). The resulting materials are likely to exhibit high Li^+-ion conductivities, while the polymeric skeleton offers a large range of options for modifying mechanical properties. Investigation of related systems of LiI with monomeric NR_4I salts. Examination of the possibility of obtaining glasses with a relatively high conductivity in which the charge carrier is a divalent cation. The target system is CdI_2-$Cd(PO_3)_2$/$Cd(PS_3)_2$. Characterizations include electrical conductivity, IR spectroscopy, internal friction and glass transition characterization.

PURDUE UNIVERSITY (continued)

438. ZERO-FLUX PLANES AND FLUX REVERSALS IN MULTICOMPONENT SYSTEMS

M. A. Dayananda - School of Materials Engineering
Phone: (317)-494-4113

$ 89,829 01-3

Interdiffusion fluxes of all components in an n-component system are calculated directly from the concentration profiles of a single diffusion couple at any section without invoking Fick's Law or the need for prior knowledge of $(n-1)^2$ interdiffusion coefficients. These studies have identified "zero-flux planes" (ZFP) for individual components, which are planes where the interdiffusion flux of a given component is zero and exhibits reversal in its flow direction on either side of the plane. Objectives include characterization of the ZFP compositions in terms of diffusion paths and thermodynamic data for multicomponent systems.

439. FORMATION OF A PARTICIPATING RESEARCH TEAM AND THE INSTRUMENTATION FOR X-RAY DIFFRACTION AT THE NATIONAL SYNCHROTRON LIGHT SOURCE (Several Institutions Involved)

G. L. Liedl - School of Materials Engineering
Phone: (317)-749-2601

$440,000 01-1

Development of an instrumented beam line and port at NSLS for conducting X-ray crystallography/diffuse scattering experiments on a variety of materials: composites, dilute metal alloys, non-stoichiometric oxides, intermetallic compounds; phenomena of interest--phase transformations, clustering, plastic deformation at crack tips; surface reactions and catalysis; overlayer structure, disordering, and melting; phonon mode softening in phase transitions.

PURDUE UNIVERSITY (continued)

440. MULTICOMPONENT DIFFUSION UNDER GENERAL CHEMICAL POTENTIAL GRADIENTS

H. Sato - School of Materials Engineering
Phone: (317)-494-4096
R. Kikuchi - School of Materials Engineering
Phone: (317)-494-4099

$ 85,884 01-3

Application of the pair approximation of the Path Probability Method (PPM) of time dependent cooperative phenomena to analytically derive the kinetic matrix of Onsager equations from thermodynamic potentials and some fundamental kinetic parameters such as jump frequencies of component atoms during multicomponent diffusion. Relations among measurable quantities and experimental concepts such as diffusion paths and zero-flux planes in multicomponent diffusion experiments and specific diffusion controlled phenomena in oxides are being investigated.

441. MECHANISMS OF ELEVATED TEMPERATURE RUPTURE IN SINGLE PHASE CERAMICS

A. A. Solomon - School of Nuclear Engineering
Phone: (317)-494-5753

$ 92,000 01-2

Study of elevated temperature tensile creep and stress rupture in well-characterized single phase ceramics in terms of rate controlling mechanisms and microstructural evolution. Experimental techniques consist of (1) tensile creep using constant true stress, (2) internal pressurization of pores with inert insoluble gas and microscopic measurement of pore or cavity growth under known hydrostatic pressure and surface tension driving forces. Results are correlated with quantitative microstructural studies of porosity evolution. Materials under investigation are CoO, UO_2, NiO and carbonyl Ni.

RENSSELAER POLYTECHNIC INSTITUTE

442. EXPERIMENTAL TESTS TO UNIFY SINTERING THEORY

R. H. Doremus - Dept. of Materials Engineering
Phone: (518)-266-6709
R. M. German - Dept. of Materials Engineering
Phone: (518)-266-6445

$ 83,000 01-1

Critical assessment of sintering theories. Measurements of particle, grain, and pore size and shape, shrinkage, surface area, and neck size during the sintering of sodium chloride, aluminum oxide, and aluminum-chromium oxide. Measurements and experimental techniques include dilatometry, buoyancy for density, scanning and transmission electron microscopy, X-ray line broadening, mercury porisometry, and BET surface adsorption.

443. PHOTON SCATTERING AND INTERACTION ANALYSIS OF INTERFACIAL CORROSION AND CATALYSIS

T. E. Furtak - Dept. of Physics
Phone: (518)-266-6454

$125,865 02-2

Develop and exploit photon scattering and interaction techniques to study fundamental and applied problems associated with corrosion and catalysis at the solid-liquid interface. Apply surface enhanced Raman scattering. Underpotential adsorption of metal monolayers on metallic substrates. Corrosion chemistry and corrosion inhibition on copper and copper alloys.

444. MOLTEN CARBONATES: MICROWAVE STUDIES OF THE VAPOR STATE

C. W. Gillies - Dept. of Chemistry
Phone: (518)-266-8453

$ 89,034 (18 months) 03-3

Characterization of the vapor state composition of lithium, sodium and potassium carbonates in the temperature range of 650-700°C by microwave spectroscopic studies. Evaluation of optimum operating parameters and electrolyte compositions in fuel cells.

RENSSELAER POLYTECHNIC INSTITUTE (continued)

445. PROTECTIVE OXIDE FILMS

R. K. MacCrone - Dept. of Materials Engineering
Phone: (518)-266-6047
S. R. Shatynski - Dept. of Materials Engineering
Phone: (518)-266-6126

$ 82,000 01-3

Study of both point defects, impurities, and grain boundaries in films of the metal oxides NiO, WO_3, and TiO_2. Techniques include both discontinuous and continuous thermogravimetric analysis, electron paramagnetic resonance, Raman spectroscopy, TEM, static magnetization, and two point electrical conductivity for the purpose of obtaining a more precise understanding of the oxidation process.

446. LOCALIZED CORROSION AND STRESS CORROSION CRACKING BEHAVIOR OF STAINLESS STEEL WELDMENTS

W. F. Savage - Materials Division
Phone: (518)-266-6780
D. J. Duquette - Materials Division
Phone: (518)-266-6490

$128,000 01-1

Corrosion of ferritic stainless steel weldments and the effect of welding parameters; chloride environments; effect of delta ferrite on localized corrosion; Cr depletion at grain boundaries; synergistic effect of sulfate and chloride ions on initiation and propagation of stress corrosion cracks; role of grain boundary precipitation; role of surface films; weldability and hot cracking of ferritic steels.

RICE UNIVERSITY

447. A STUDY OF THE KINETICS AND THERMODYNAMICS OF HYDROGEN IN Pd-BASED ALLOYS

R. B. McLellan - Dept. of Mechanical Engineering & Materials Science
Phone: (713)-527-4993

$ 50,175 01-3

Systematic measurements of the solubility, thermodynamic properties, and diffusivity of H atoms in the same Pd-based binary alloys. Low (270-350K) and high (500-1000K) temperature diffusion measurements respectively by a double-cell electrolyte system and the permeability time-lag method. Measurement of the temperature and pressure dependence of hydrogen solubility and the temperature and the substitutional solute concentration dependence of the elastic constants. Theoretical investigation of low temperature effects and for H diffusion in Fe. Magnetic susceptibility and elastic constant measurements for Pd and Pd alloys. Statistical thermodynamic modelling.

448. ELECTRON SPIN POLARIZATION EFFECTS IN LOW ENERGY ELECTRON DIFFRACTION, ION NEUTRALIZATION AND METASTABLE ATOM DEEXCITATION AT SOLID SURFACES

G. K. Walters - Dept. of Physics
Phone: (713)-527-4937
F. B. Dunning - Dept. of Physics
Phone: (713)-527-8101

$179,724 02-2

Will use PLEED (polarized LEED) to study surfaces; e.g., Ni with Te adsorbed and W with H absorbed. Spin polarization measurements in conjunction with ion neutralization spectroscopy (INS) and metastable deexcitation spectroscopy (MDS) to study surface electronic structure on magnetic materials such as Ni. Polarized He$^+$ beams used for INS and polarized He (2^3S) beams for MDS.

UNIVERSITY OF ROCHESTER

449. FRACTURE TOUGHNESS PROCESSES

S. J. Burns - Dept. of Mechanical and Aerospace Sciences
Phone: (716)-275-4082

$ 80,000 01-2

Studies of macro-tip dislocation plasticity and the production of microcracks. Materials under investigation include aluminum alloys, various steels, silicon and a number of oxide ceramics. Types of measurements include (a) dislocation nucleation and structures at the tips of cracks, (b) the relationship between positions of dislocations relative to crack-tips and the stress intensity factor for crack propagation, and (c) transmission electron microscopy of dislocations at crack tips.

450. DIFFUSIONAL CREEP OF MULTICOMPONENT SYSTEMS

J. C. M. Li - Dept. of Mechanical and Aerospace Engineering
Phone: (716)-275-4038

$106,764 01-2

Stress-motivated diffusion; elastic and plastic deformation in ceramic, polymer, and metallic materials; techniques - "impression" creep, fatigue, load relaxation, and elastic deformation; relationships between bulk and impression test data; polycrystals and single crystals; laser excited solid-state reactions, plasticity, and diffusion; Al, β-tin, LiF, KCl, Nb.

ROCKWELL INTERNATIONAL SCIENCE CENTER

451. SINTERING PHENOMENA OF NON-OXIDE SILICON COMPOUNDS

F. F. Lange, T. M. Shaw, P. E. D. Morgan
Phone: (805)-498-4545

$194,982 01-1

Evaluation of the influence of new colloidal precipitation and conventional powder preparation methods for the preparation of Si_3N_4 powder on the microstructure and microchemistry of both green and sintered compacts. Development of a colloidal method for preparing Si_3N_4 synthesis materials by investigating the slip casting of colloidally mixed slips. Study of the Si-S-N chemistry for the synthesis of Si_3N_4 powder. Techniques to obtain a homogeneous distribution of sintering aids and their effect on the resultant microstructure and microchemistry. Development of quantitative methods based on X-ray microanalysis and backscattered electron imaging, for gauging compositional uniformity of powder compacts and sintered materials.

RUTGERS UNIVERSITY

452. METAL ATOM DIFFUSION IN AMORPHOUS SILICA AND AT THE SILICA SURFACE

S. H. Garofalini - Dept. of Ceramics
Phone: (201)-932-2216

$ 67,000 01-3

Bulk and surface diffusion studies in amorphous silica with the objective of understanding the effects of local structure, interatomic forces, and atom size. Molecular dynamics computer simulation studies in conjunction with EXAFS and SAXS experiments using metal species in bulk amorphous silica. Molecular dynamics computer studies of adatom species in bulk amorphous silica. Molecular dynamics computer studies of adatom species Pd, Pt, or Ag on amorphous silica surfaces to determine the effects of local structure. Specimen preparation by sol-gel processes.

453. HIGH PRESSURE ELECTRON RESONANCE STUDIES OF ELECTRONIC, MAGNETIC AND STRUCTURAL PHASE TRANSITIONS

J. H. Pifer - Dept. of Physics
Phone: (201)-932-2522
M. C. Croft - Dept. of Physics
Phone: (201)-932-2524

$122,000 02-2

Develop high pressure diamond anvil cell in which to make electron paramagnetic resonance measurements. Use this apparatus to study phase transitions in phosphorus doped silicon, organic charge transfer salts, europium compounds and cesium.

UNIVERSITY OF SOUTHERN CALIFORNIA

454. LIMITING PROCESSES IN LASER CVD

S. D. Allen - Center for Laser Studies
Phone: (213)-743-6705
S. Copley - Center for Laser Studies
Phone: (213)-743-6223

\$126,468 01-5

Experimental and theoretical research with the objective of developing an understanding of the laser chemical vapor deposition (LCVD) process sufficient to predict deposition rates, microstructures, and resulting film properties. Predictions will account for the effects of surface temperature, laser spot size, local vapor composition, total pressure, optical absorption, thermal properties and thermal expansion mismatch. These variables are to be isolated by means of experiments designed to measure chemical, optical, thermal and mechanical effects. Calculations and measurements of surface temperature and theoretical analysis of convective and diffusive transport correlated with experimental results. Model system: SiC deposited by two types of reactions on various substrates will be investigated to study chemical and transport effects. LCVD of SiC on Mo coated SiC substrate will be used to investigate the effect of changes in optical properties during LCVD. Changes in both optical and thermal properties during LCVD studied by depositing SiC on Mo substrates. Residual interface stresses and their role in LCVD film adherence investigated by depositing SiC on W substrates. Characterization of film thickness profiles, microstructures and film adherence.

455. ELECTRICAL AND MECHANICAL PROPERTIES OF OXIDE CERAMICS

F. A. Kröger - Dept. of Materials Science
Phone: (213)-743-6224

\$132,000 (17 ½ months) 01-3

Relationship between the composition and microstructure with physical behavior of oxide ceramics, principally Al_2O_3. Relationship of composition, including non-stoichiometry, and microstructure to dopants, conditions of preparation, oxygen fugacity, and temperature, and their effect on physical properties through the defect structure. Experimental studies include electrical conductivity, emf measurements on concentration cells to determine partial ionic and electrical conductivities, electron-spin resonance, optical absorption, and creep.

UNIVERSITY OF SOUTHERN CALIFORNIA (continued)

456. GRAIN BOUNDARY SLIDING AND DEFORMATION MECHANISMS DURING HIGH TEMPERATURE CREEP

T. G. Langdon - Dept. of Materials Science and Mechanical Engineering
Phone: (213)-741-2095

$125,000 01-2

Measurement of creep and grain boundary sliding in metals; boundary sliding, stress and temperature dependences, threshold creep stress in precipitation hardened and solid solution strengthened Al-base alloys; boundary migration under monotonic as well as cyclic creep; cavitation in Cu alloys and Pb.

SOUTHERN ILLINOIS UNIVERSITY

457. METALLIC GLASSES AND NON-EQUILIBRIUM PHASES AS NEW CATALYSTS IN ENERGY CONVERSION SYSTEMS

W. E. Brower, Jr. - Dept. of Engineering Mechanics and Materials
Phone: (618)-536-2368
G. Smith- Dept. of Chemistry and Biochemistry
Phone: (618)-453-5721

$ 77,000 01-1

Identification of the catalytic activity of non-equilibrium crystalline and amorphous metals, specifically Pd- and Ni-base alloys, and the role of defects thereon; characterization of microstructure and transformation kinetics of rapidly-cooled alloys; use of molecular probe.

SOUTHWEST RESEARCH INSTITUTE

458. THE STUDY AND MODELLING OF HIGH TEMPERATURE FATIGUE CRACK PROPAGATION IN AUSTENITIC STAINLESS STEEL

D. L. Davidson - Dept. of Materials Sciences
Phone: (512)-684-5111

$ 45,000 01-2

In-situ observation of crack tip strain fields in austenitic stainless steels under creep and creep-fatigue loading, and correlation with microstructural features; techniques used: SEM, electron channeling, and optical stereo imaging.

SOUTHWEST RESEARCH INSTITUTE (continued)

459. CHARACTERIZATION AND ANALYSIS OF CAVITY DEVELOPMENT DURING CREEP OF CERAMICS AT ELEVATED TEMPERATURES

R. A. Page - Dept. of Materials Science
Phone: (515)-684-5111, x3252
J. Lankford - Dept. of Materials Sciences
Phone: (515)-684-5111, x2317

$ 80,148	01-2

Determination of cavity nucleation and growth rates as a function of (incubation) time, applied compressive stress, and microstructure during the early stages of creep in Al_2O_3 and SiC. Cavitation creep modelling. This experimental research is based on the use of the 30m SANS (small angle neutron scattering) instrument at ORNL with measurements to be performed over the angular range $5x10^{-3}\,\text{Å}^{-1} \leq q \leq 3.5x10^{-2}\,\text{Å}^{-1}$ with neutrons of wavelength 4.75Å and an angular resolution of approximately $1x10^{-3}\,\text{Å}^{-1}$. SANS data will be reduced to yield the radius of gyration, Porod radius total cavity surface area, total cavity volume, and total cavity number. Density measurements by a sink-float technique on a specimen suspended within a temperature-controlled pycnometer. Dark field and lattice fringe imaging electron microscopy.

STANFORD UNIVERSITY

460. PHOTOELECTRONIC PROPERTIES OF II-VI HETEROJUNCTIONS

R. H. Bube - Dept. of Materials Science and Engineering
Phone: (415)-497-2534

$187,094	01-3

Interactions occurring at the interface between CdTe with other materials, and the role of interfacial microstructure and microchemistry on the electrical properties of such CdTe containing heterojunctions. Effects of etching and heat treatment on surfaces, Schottky barriers, and heterojunctions formed on CdTe, and the preparation and behavior of polycrystalline films of CdTe. Grain boundary characterization and passivation. Measurements include J-V curves in dark and light; junction capacitance; surface photovoltage; Schottky-barrier formation; spectral response; and diffusion lengths. Scanning transmission electron microscopy and high resolution TEM analysis of heterojunction interfaces; lattice resolution; electron microdiffraction; XPS, Auger analysis; vacuum evaporation; spray pyrolysis; rf sputter deposition, magnetron sputtering, and chemical vapor deposition, and closed-space vapor transport techniques.

STANFORD UNIVERSITY (continued)

461. EVALUATION OF MACHINING DAMAGE IN BRITTLE MATERIALS

B. T. Khuri-Yakub - Dept. of Electrical Engineering
Phone: (415)-497-0718

$102,600 01-5

NDE measurement of cracks and residual stress induced by machining ceramics, initially Si_3N_4, and a model brittle material, Si; crack size determination with acoustic and laser techniques, and residual stress level with acoustic methods.

462. MODELLING OF DEFORMATION AND FRACTURE IN HIGH-TEMPERATURE STRUCTURAL MATERIALS

A. K. Miller - Dept. of Materials Science and Engineering
Phone: (415)-497-3732

$172,200 01-2

Development of quantitative methods of predicting deformation and fracture of metals and alloys subjected to complex histories and environments; computer based constitutive equations for non-elastic-deformation, "MATMOD"; modelling of fatigue crack initiation and growth, "FATIGMOD"; modelling of multiaxial plastic flow; applications to Type 304 stainless steel, 2 1/4 Cr-1 Mo steel and Al alloys.

463. THE USE OF SURFACE ACOUSTIC WAVES TO STUDY SMALL FATIGUE CRACKS

D. V. Nelson - Dept. of Mechanical Engineering
Phone: (415)-497-2123
J. C. Shyne - Dept. of Materials Science and Engineering
Phone: (415)-497-2535

$124,300 01-5

Investigation of fatigue crack growth in austenitic stainless and martensitic low alloy steels, using surface acoustic waves as a probe of crack depth and closure stress; influence of crack tip plasticity on acoustic method; correlation of crack propagation rate, crack closure stress, and cyclic stress ratio.

STANFORD UNIVERSITY (continued)

464. A STUDY OF THE MICROSTRUCTURAL PROCESSES WHICH CONTROL HIGH TEMPERATURE CRACK GROWTH

W. D. Nix - Dept. of Materials Science and Engineering
Phone: (415)-497-4259

$ 80,397 01-2

Study of creep deformation, cavitation, and cracking in metals (Cu and Ni) with either impurity segregation or with an array of gas bubbles at grain boundaries; stress field at creep crack tips; correlation of crack growth with grain size, degree of segregation, and creep deformation parameters; identification of mechanisms controlling creep crack growth.

STEVENS INSTITUTE OF TECHNOLOGY

465. STUDIES OF MAGNETISM AND EXCHANGE SCATTERING IN SOLIDS USING SYNCHROTRON RADIATION AND SPIN POLARIZED PHOTOELECTRONS

G. M. Rothberg - Dept. of Materials and Metallurgical Engineering
Phone: (201)-420-5269

$ 84,000 02-2

A synchrotron light source will be used to produce polarized photoelectrons from transition metal ions. The multiplet splitting serves as the polarizer. Spin polarized EXAFS will be used to study instantaneous short range magnetic order above and below transition temperatures and on surfaces and to study temperature dependence of short range order above transition temperatures.

SYRACUSE UNIVERSITY

466. THE CATALYTIC REACTIVITY OF CRYSTAL SURFACES

R. W. Vook - Dept. of Chemical Engineering and Materials Science
Phone: (315)-423-3466

$119,000 01-1

Characterization of topography of thin single crystal metal films (Pd, Pt); measurement of the adsorption kinetics of O_2, CO, and hydrocarbons on these films; identification of film growth mechanism; correlation of film defect structure with adsorption behavior; relation of above to catalytic activity; techniques used - LEED, AES, EELS.

UNIVERSITY OF TEXAS

467. POLAR FLUIDS: PHOTOEMISSION AND ELECTRONIC ENERGY LEVELS

J. C. Thompson - Dept. of Physics
Phone: (512)-471-5926
P. R. Antoniewicz - Dept. of Physics
Phone: (512)-471-3766

$ 90,009 02-2

Measure photoinjected current in polar fluids (NH_3, H_2O and alcohols) as a function of bias, photon energy and temperature. Ag electrode illuminated by pulsed dye laser. Measure i-V curves and determine electronic energy levels, interfacial work functions. Concurrent theoretical work includes calculation of density of states.

UNIVERSITY OF UTAH

468. MULTI-SPECTROSCOPIC STUDIES OF THE ELECTRONIC STRUCTURE OF ELECTRODE MATERIALS FOR HIGH ENERGY DENSITY BATTERIES: I-II AND I-III INTERMETALLIC COMPOUNDS WITH B32 STRUCTURE

I. M. Curelaru - Dept. of Materials Science and Engineering
Phone: (801)-581-3589

$ 75,000 01-1

Systematic investigation of the electron structure of the occupied and empty states for I-II and I-III intermetallic Zintl compounds, with concern for the significance of non-stoichiometry, defect lattice, and degree of localization of conduction orbitals in determining physical behavior. Spectroscopic techniques consist of X-ray photoelectron spectroscopy (XPS), electron energy loss spectroscopy (EELS), core ionization loss spectroscopy (CILS), appearance potential spectroscopy (APS), and extended appearance potential fine structure (EAPFS). Comparison of XPS, EELS, CILS, and APS data with existing LCAO, cluster model, and self-consistent linear muffin-tin LMT band-structure calculations.

UNIVERSITY OF UTAH (continued)

469. THEORETICAL AND EXPERIMENTAL STUDY OF SOLID PHASE MISCIBILITY GAPS IN III/V QUATERNARY ALLOYS

G. B. Stringfellow - Depts. of Materials Science and Engineering
and Electrical Engineering
Phone: (801)-581-8387 -

$ 66,426 01-3

Miscibility gap studies in III-V quaternary alloys, including (1) development of models and techniques for calculating solid-solid miscibility gaps in quaternary alloys, (2) calculation of effects of coherency strain on the equilibrium phase diagram, (3) experimental determination of the miscibility gap in the system $Ga_xAl_{1-x}As_{1-y}Sb_y$ in both homogeneously nucleated platelets (without elastic strain) and liquid phase epitaxial layers on GaAs and InP substrates, (4) calculating the effects of elastic strain in epitaxial growth, and (5) miscibility study of $Ga_xAl_{1-x}As_{1-y}Sb_y$ alloys grown by the kinetically controlled organometallic vapor phase epitaxial technique. Investigation for nonequilibrium alloys of spinodal decomposition and its effects on the electrical and optical properties of the alloys. STEM and X-ray analysis.

VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY

470. FRACTURE MECHANISMS IN GLASS-CRYSTAL COMPOSITES

D. P. H. Hasselman - Dept. of Materials Engineering
Phone: (703)-961-5402

$ 99,392 (17 months) 01-2

Fracture mechanisms in glass-crystal composites with a cordierite glass-ceramic and its original (non-crystallized) glass as the principal materials of study. Flaw introduction by micro-hardness indentation and crack characterization by scanning electron microscopy. Characterization of localized stress distribution near crystalline dispersions, sub-critical and critical crack propagation behavior, associated crack-crystalline interaction, and mechanisms which control the nature (size, geometry) of the fracture-initiating flaw. Biaxial flexure and double torsion or double cantilever beam strength characterizations. Environmental and loading conditions include ambient room air and inert environments, and variable loading rates to establish strain-rate sensitivity.

VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY (continued)

471. HYDROGEN EMBRITTLEMENT TESTING

M. R. Louthan, Jr. - Dept. of Materials Engineering
Phone: (703)-961-6640

$ 25,000 01-2

Evaluation of the effective H_2 fugacity in electrochemically-charged steels by comparison with gaseous permeation data; mechanical testing of carbon and low alloy steels either electrochemically charged or in gaseous hydrogen up to 65 MPa; effect of chemical poisons on H_2 ingress; influence of pre-existing flaws on susceptibility to embrittlement.

UNIVERSITY OF VIRGINIA

472. SPECTROSCOPY OF SURFACE ADSORBED MOLECULES

R. V. Coleman - Dept. of Physics
Phone: (804)-924-3781

$ 96,000 02-2

Investigations of the properties of surfaces and interfaces containing molecular adsorbates using inelastic electron tunneling (IETS), photoemission (ESCA), and Auger spectroscopies. IETS spectra will be obtained for a number of combinations of oxide substrate and metal overlayer electrodes to establish the nature of the chemical and electronic interactions between molecules and interface. ESCA and Auger studies will be made on the same systems to augment the IETS work. Studies of UV-induced damage to molecules and photocatalytic effects on semiconductor oxides.

473. MAGNETIC IMPURITIES IN SUPERCONDUCTORS

J. Ruvalds - Dept. of Physics
Phone: (804)-924-3782

$ 80,057 02-3

Theoretical research on magnetic impurity interactions in superconductors. Study of rare earth impurities in various metallic hosts to determine relative importance of exchange interactions and to examine electronic structural basis for coupling. Studies on influence of impurities, at intermediate concentrations, on the electron spin susceptibility and nuclear spin relaxation rate. Continuing emphasis on investigating new mechanisms for achieving enhancement of superconducting properties in high magnetic fields.

UNIVERISTY OF VIRGINIA (continued)

474. THE EFFECT OF MICROSTRUCTURE ON THE FATIGUE BEHAVIOR OF Fe-C-X ALLOYS

E. A. Starke - Materials Science Dept.
Phone: (804)-924-7097
G. J. Shiflet - Materials Science Dept.
Phone: (804)-924-6340

$ 60,500 (15 months) 01-2

Experimental correlation of fatigue behavior of duplex martensitic-ferritic steels with microstructural features such as carbide type, morphology and distribution, and continuity of ferrite vs. martensite; crack initiation and propagation in high and low cycle fatigue; crack cloture effects.

UNIVERSITY OF WASHINGTON

475. NUCLEAR MAGNETIC RESONANCE STUDIES OF ION MOTION IN SOLID ELECTROLYTES

J. L. Bjorkstam - Dept. of Electrical Engineering
Phone: (206)-543-2177

$ 89,205 01-3

Nuclear magnetic resonance (NMR) studies of spin-spin and spin-lattice relaxation times, effects of motion and structure upon the electric quadrupole NMR spectrum, and direct NMR diffusion measurements to study the solid electrolytes mixed cation β-alumina, phosphoborate glasses, and lithium iodide monohydrate. Correlative studies involve electrical conductivity and thermal analysis. Temperature and frequency dependence of the spin-lattice relaxation to understand ion-ion and ion-lattice interactions and predict electrolyte systems with optimized conductivity. Other techniques invoked include thermogravimetric analysis, X-ray diffraction, infrared absorption, thermomodulated uv-reflectivity and thermoelectric currents.

476. RUBBER ELASTICITY

B. E. Eichinger - Dept. of Chemistry
Phone: (206)-543-1653

$ 151,270 (24 months) 03-1

Experimental studies of the elastic contribution to the chemical potential of a swelling agent in crosslinked and uncrosslinked polydimethlsiloxane. Theoretical studies on eigenvalue spectra of Kirchoff matrices which describe random networks. Characterization using small angle X-ray scattering.

UNIVERSITY OF WASHINGTON (continued)

477. X-RAY SPECTROSCOPY OF SOLIDS UNDER PRESSURE

R. L. Ingalls - Dept. of Physics
Phone: (206)-543-2778

$ 70,000 02-2

Investigate the structure and behavior of materials at high pressure by pressure-sensitive phase transformations. The X-ray absorption near-edge structure (XANES) is utilized on material exhibiting structural or thermal disorder-liquid metals and layered compounds.

UNIVERSITY OF WEST VIRGINIA

478. ELECTRON HYBRIDIZATION EFFECTS AND THE CRYSTAL STRUCTURE OF PLUTONIUM

B. R. Cooper - Dept. of Physics
Phone: (304)-293-3423

$ 56,953 03-1

Theoretical studies of the crystallographic allotropic transformations of elemental plutonium. Band calculations of the electronic structure, lattice energy, and correlation effects for plutonium and plutonium compounds.

UNIVERSITY OF WISCONSIN/MILWAUKEE

479. MICROSTRUCTURAL ANALYSIS OF ION-CONTAINING POLYMERS

S. L. Cooper - Dept. of Chemical Engineering
Phone: (608)-262-3641

$ 82,820 03-1

Studies of microstructure of several ionomer systems by SAXS, EXAFS and Mössbauer spectroscopy. Characterization of size and separation of ionic domains using correlation function derived from small angle X-ray scattering measurements. Investigations of relationships between composition and preparation variables and morphology and transport properties.

UNIVERSITY OF WISCONSIN/MILWAUKEE (continued)

480. INTERACTION OF LOW ENERGY ELECTRONS WITH SURFACE LATTICE VIBRATIONS

S. Y. Tong - Dept. of Physics and Surface Studies Laboratory
Phone: (414)-963-4474

$ 74,985 02-2

Theory of electron energy loss spectroscopy (EELS) of surfaces. Vibrational properties of isolated adatoms and ordered overlayers on metal surfaces, with emphasis on quantitative comparisons with experiment. Role of image potential in large-angle EELS and in LEED studies. Large-angle inelastic scattering from substrate phonons. EELS spectral densities at large wave vector. Surface relaxation, anharmonicity, and surface lattice dynamics. This program strongly coupled to that of D. L. Mills, University of California-Irvine.

UNIVERSITY OF WISCONSIN/MADISON

481. INVESTIGATION OF AMORPHOUS METAL FILMS ON SEMICONDUCTOR SUBSTRATES

J. D. Wiley - Dept. of Electrical and Computer Engineering
Phone: (608)-263-2354, 1643
J. H. Perepezko - Dept. of Metallurgy and Mineral Engineering
Phone: (608)-263-1678

$ 75,000 01-1

Experimental investigation of the structure, stability, and atomic transport behavior of high-T_g amorphous-metal films on semiconductor substrates. RF sputtering deposition of thin amorphous films of Ni-Nb, Mo-Si, and W-Si alloys on semiconductor substrates of Si, GaAs, and GaP. Characterization of crystallization kinetics, crystallization mechanism, and film/substrate interdiffusion at temperatures near the glass-transition temperature by structural, calorimetric, and electrical measurements. Examination of structural relaxation by electrical resistivity measurements during post-deposition annealing. Measurement of diffusion and interdiffusion by a combination of Rutherford back scattering and Auger electron spectroscopy techniques. Assessment of reactions involving crystallization and possible phase separation, involving TEM analysis of in-situ annealing, and supplementary SEM and X-ray diffraction measurements.

UNIVERSITY OF WISCONSIN/MADISON (continued)

482. OPTICAL STUDIES OF DYNAMICAL PROCESSES IN DISORDERED MATERIALS

W. M. Yen - Dept. of Physics
Phone: (608)-263-7475

$ 80,000 (6 months) 02-2

This program is a comprehensive study of relaxation and energy transfer properties of optically-active disordered systems and exploratory investigations of doped ceramics. A capability to measure coherent transient effects will be developed to be used in conjunction with an existing facility for Fluorescence Line Narrowing. The first component of this program will investigate the temperature dependence of the relation effects in disordered materials and testing of disordered materials will be investigated to determine the microscopic interactions and to extend the models. The third phase will be a fundamental study of ion transfer, trapping, and cross relaxation in a prototypical glass system.

SECTION C

Small Business Innovation Research

This information was prepared by the DOE-Division of Materials Sciences project manager. All projects are Phase I, with the goal to determine, insofar as possible, the scientific or technical merit and the feasibility of ideas submitted under the SBIR program. Phase I funding is limited to less than $50,000 per project for a period generally of less than six months.

ALTEX CORPORATION

500. EXTREME ULTRAVIOLET AND SOFT X-RAY INSTRUMENTATION FOR MICROCHARACTERIZATION OF MATERIALS

H. Pummer
(312)-996-7499

SBIR

The objective of the proposed research program is to quantify the key factors which determine performance, complexity, and cost of an excimer laser system for the generation of coherent high spectral brightness radiation in the extreme ultraviolet and soft x-ray spectral regions. The first phase of this research effort will center on the critical issue of the generation of a high quality picosecond seed beam suitable for amplification in excimer lasers. The efficiency of different frequency conversion schemes and the characteristics of various pulse slicing techniques will be studied. Finally, a feasibility and cost study for a commercial picosecond excimer laser system suitable for short wavelength generation will be performed.

CERAMIC FINISHING COMPANY

501. FRACTURE MECHANICS INVESTIGATION OF GRINDING OF CERAMICS

H. P. Kirchner
(814)-238-4270

SBIR

Application of contact fracture mechanics to investigate mechanisms of material removal and damage penetration during abrasive machining of ceramics. In Phase I it is planned to emphasize investigation of the mechanisms of material removal including crushing by mixed mode fracture ahead of the diamond point and chipping at lateral cracks propagating in response to residual stresses induced by elastic relaxation against the irreversibly deformed zone on unloading. The objective is to determine the relative importance of crushing ahead of the diamond point and chipping alongside the track as a result of lateral cracking, for various material properties and grinding conditions. The role of crushing in reducing the residual stresses that are responsible for lateral cracking will be investigated. Mathematical models will be developed by adapting available models for static indentations. The experimental results will be compared with results predicted by these models.

CERES CORPORATION

502. HORIZONTAL GROWTH OF SILICON SHEET CRYSTALS VIA EDGE-SUPPORTED PULLING (ESP) FROM A MELT CONTAINED IN A COLD CRUCIBLE

J. F. Wenckus
(617)-899-5522

SBIR

The program will explore the feasibility of growing silicon sheet crystals horizontally using the edge-supported pulling (ESP) process from silicon melts contained in an RF heated crucible. The vertical edge-supported pulling (ESP) process provides exceptionally stable sheet growth conditions. However, the sheet growth rates achieved to date are severely restricted by the rate of heat dissipation from the narrow sheet/melt interface. Moreover, since the filaments in the ESP process pass through holes in the bottom of the melt container, shallow melt levels must be used and melt replenishment during growth has yet to be achieved. This program will endeavor to integrate the unique operational features of the cold crucible with the equally unique attributes of the ESP process in order to demonstrate the feasibility of the horizontal edge-supported pulling (HESP) method for the production of silicon crystals.

ELECTROCHEMICAL TECHNOLOGY CORPORATION

503. MATHEMATICAL MODELING OF STRESS CORROSION CRACKING

T. R. Beck
(206)-632-5965

SBIR

Mathematical modeling of the electrochemical transport and kinetic processes that occur in tunnel corrosion of aluminum; correlative experiments on salt film properties using the shielded electrode technique; relation of the above to stress corrosion cracking.

FIBER MATERIALS, INC.

504. HIGH PERFORMANCE SILICON CARBIDE AND SILICON NITRIDE

H. D. Batha
(207)-282-5911, x280

SBIR

Hot isostatic pressing (HIPing) of silicon nitride and silicon carbide in nitrogen in order to define operating conditions, raw material properties and the role of certain additives required to produce bodies with superior strength and toughness. Investigation of the role of microstructural acicular SiC or Si_3N_4 on strengthening and the formation of ceramic fiber reinforced ceramics.

MEASUREMENT CONCEPTS, INC.

505. DEVELOPMENT OF A SINGLE APERTURE-FOUR CHANNEL NANOSECOND POLARIMETER FOR APPLICATION TO THE NON-DESTRUCTIVE EVALUATION (NDE) OF MATERIALS

E. Collett
(201)-780-7576

SBIR

The design and fabrication of a new type of polarimeter called a Single Aperture-Four Channel Optical Polarimeter will be undertaken. It is designed to measure simultaneously the four Stokes polarization parameters of an optical beam and is capable of measuring the Stokes parameters of either a cw or pulsed optical beam and is readily adapted to ellipsometry. If a dielectric film is illuminated with a single pulse of right or left circularly polarized light then the index of refraction and the thickness of the thin-film can be found non-destructively.

SUPERCON, INC.

506. AN INVESTIGATION TO DETERMINE THE COMMERCIAL FEASIBILITY OF IN SITU Cu-Nb COMPOSITES FOR HIGH STRENGTH, HIGH CONDUCTIVITY APPLICATIONS

J. Wong
(617)-655-0500

SBIR

Development of a procedure for determining the commercial feasibility of fabricating in situ Cu-Nb multifilamentary composites for high stress, high conductivity applications; maintenance of a low volume fraction of Nb to retain desirable electrical and thermal properties of Cu; evaluation of composite formability, tensile and fatigue strengths, and electrical conductivity.

TECHNOLOGY FOR ENERGY CORPORATION

507. A HIGH-SPEED, CURVED, POSITION-SENSITIVE X-RAY DETECTOR

R. W. Hendricks
(615)-966-5856, x2524

SBIR

A new high-speed, curved position-sensitive x-ray detector will be developed. The design will circumvent several of the limitations of current linear position-sensitive detectors. The unique features of the proposed detector are: multiple anode wires in a unique spacing arrangement which will distribute the space charge over a wider area and will lead to both longer detector lifetime and higher count-rate capability; and a new concept for a planar fan-shaped cathode wire meander which allows both finer wire spacings and higher resistance and thus high spatial resolution on a curved array.

UNIVERSAL ENERGY SYSTEMS, INC.

508. FABRICATION OF AMORPHOUS METALLIC FILMS AND COATINGS FOR INDUSTRIAL APPLICATIONS USING HIGH ENERGY ION BEAM MIXING

P. P. Pronko
(513)-426-6900

SBIR

Fabrication of amorphous Ni- and Cu-base metallic films and coatings using deeply penetrating high energy ion beam mixing; use of the so-called structural difference rule for amorphous alloy formation by ion mixing; evaluation of modified surfaces in erosive and corrosive pitting conditions, e.g. involving exposure to electro-hydrodynamic and corrosive fluid dynamic environments; comparison with crystalline metal behavior.

SECTION D

Collaborative Research Centers

Basic materials research which is long range, generic in nature, is conducted by the Office of Basic Energy Sciences/Division of Materials Sciences to provide an underpinning for the development of energy systems. In the pursuit of these research goals, facilities or centers which are unique and/or expensive and costly to reproduce elsewhere have been and are being developed. Scientists from other laboratories outside of the host laboratory are encouraged to make use of these unique facilities. In this section, a description is included for a number of the most important centers together with a statement of the method of gaining access to them. The collaboration carried out by outside users has to be in the furtherance of DOE objectives. Any activity which can be carried out through commercially available laboratories is not appropriate for these DOE centers. In addition, proprietary research cannot be conducted unless there is full cost recovery. Each center has a slightly different mode of operation tailored to its best use. For more information, it is recommended that the reader make use of the laboratory contacts listed.

NATIONAL SYNCHROTRON LIGHT SOURCE

Brookhaven National Laboratory
Upton, New York 11973

The National Synchrotron Light Source (NSLS) facility consists of a 750 MeV (9 electron bunch) storage ring for VUV and IR research and a 2.5 GeV (30 electron bunch) storage ring for X-ray research. Attractive features of the synchrotron radiation include high brightness and intensity, its broad and continuous spectral range, high polarization and pulsed time structure (subnanosecond pulses). With each of the 28 X-ray and 16 VUV beam ports being further split into from 2 to 4 beam lines, it will be possible to have as many as 100 experiments running simultaneously at the NSLS. A 6 pole superconducting wiggler magnet and a 38 pole permanent magnet undulator have been constructed, and several wiggler and undulator magnets are presently being designed which will significantly increase the photon intensity and brightness.

The NSLS is a facility where a wide range of research techniques will be utilized by biologists, chemists, solid state physicists, metallurgists, and engineers for basic and applied studies. Among the techniques are EXAFS (extended X-ray absorption fine structure), scattering, diffraction, topography, radiography, fluorescence, interferometry, gas phase spectroscopy, photoemission, radiometry, lithography, microscopy, dichroism, and infrared vibrational spectroscopy.

USER MODE

The policy for experimental utilization of the NSLS is designed to enable the scientific community to cooperate in the design and fabrication of experimental apparatus. In addition to the beam lines constructed by the NSLS staff for general usage, a large number of beam lines are being designed and instrumented by "Participating Research Teams" (PRTs). The PRTs are given priority for up to 75% of their beam line(s) operational time for a three-year term.

General Users will be able to perform experiments on an NSLS facility beam line or on a PRT beam line which will be available for use by non-PRT members for at least 25% of its total operational time. In the latter case, PRTs will provide liaison and utilization support to General Users. After an initial commissioning period, NSLS and PRT beam lines will become available for use by General Users.

Proprietary research can be performed at the NSLS. A full-cost recovery fee will be charged for the amount of beam time utilized. The DOE has granted the NSLS a Class Waiver, under the terms of which Proprietary Users of the NSLS will have the option to retain title to inventions that result from research performed at the Light Source.

A limited amount of funding will be available to scientists from U.S. institutions of higher education under the NSLS-HFBR Faculty/Student Support Program. The program is designed to defray expenses incurred by faculty/student research groups performing experiments at the NSLS or at the HFBR. It is aimed at university users having only limited grant support for their research, and will be used to support only the most deserving cases.

PERSON TO CONTACT FOR INFORMATION

R. Klaffky	(516) 282-4974
NSLS - Bldg. 510E	(FTS) 666-4974
Brookhaven National Laboratory	
Upton, New York 11973	

NATIONAL SYNCHROTRON LIGHT SOURCE

TECHNICAL DATA

Facilities	Key Features	Operating Characteristics
VUV electron storage ring	high brightness, continuous wavelengh range (λ > 5 Å) 16 beam ports.	0.75 GeV electron energy
X-ray electron storage ring	high brightness, continuous wavelength range (λ > .5 Å) 28 beam ports	2.5 GeV electron energy
Instruments		
Monochromators:		
plane grating	12 Å < λ < 1500 Å; high resolution	
zone plate	8 Å < λ < 100 Å; moderate resolution	
toroidal grating	10 Å < λ < 2500 Å; high intensity, moderate and high resolution	
extended range grasshopper	20Å < λ < 2000Å; high resolution	
Wadsworth	300 Å < λ < 3000 Å; high intensity, moderate resolution	
Seya & Czerny Turner	1200 Å < λ < 12000 Å; high intensity, moderate resolution	
two crystal	.04 Å < λ < 2500 Å; high resolution, fixed exit beam	
two crystal/two grating	2.5 Å < λ < 2500 Å; high resolution, fixed exit beam	
Six circle spectrometer/ diffractometers	high positional and rotational accuracy	
Experimental stations	photoemission, magnetic circular dichroism, fluourescence, gas phase spectroscopy, microscopy, lithography, holography, EXAFS, inelastic scattering, crystallography, radiometry, topography, small angle scattering	
Superconducting wiggler	λ > .1 Å; high intensity	
Permanent magnet undulator	100 Å < λ < 1000 Å; high intensity and brightness	

HIGH FLUX BEAM REACTOR

Brookhaven National Laboratory
Upton, New York 11973

The Brookhaven High Flux Beam Reactor (HFBR) operates at a power of 60 megawatts and provides an intense source of thermal neutrons (total thermal flux = 1.0×10^{15} neutrons/cm^2-sec). The HFBR was designed to provide particularly pure beams of thermal neutrons, uncontaminated by fast neutrons and by gamma rays. A cold source (liquid hydrogen moderator) provides enhanced flux at long wavelengths ($\lambda > 4$ Å). A polarized beam spectrometer, triple-axis spectrometers and small-angle scattering facilities are among the available instruments. Special equipment for experiments at high and low temperatures, high magnetic fields, and high pressure are also available. The emphasis of the research efforts at the HFBR has been on the study of fundamental problems in the fields of solid state and nuclear physics and in structural chemistry and biology.

USER MODE

The HFBR serves the U.S. scientific community and there exists a strong collaboration between the Brookhaven staff and users from universities, industry, and other national laboratories. In 1982 more than 160 persons from outside institutions participated in experiments at Brookhaven. Experiments are scheduled at the HFBR following review of research proposals. Please contact R. Klaffky for more information and for a copy of the HFBR Handbook which contains considerable detail on the available equipment and on operating procedures.

A limited amount of funding will be available to scientists from U.S. institutions of higher education under the NSLS-HFBR Faculty/Student Support Program. The program is designed to defray expenses incurred by faculty/student research groups performing experiments at the National Synchrotron Light Source or at the HFBR. It is aimed at university users having only limited grant support for their research, and will be used to support only the most deserving cases.

PERSON TO CONTACT FOR INFORMATION

R. Klaffky (516) 282-4974
NSLS - Bldg. 510E FTS 666-4974
Brookhaven National Laboratory
Upton, New York 11973

HIGH FLUX BEAM REACTOR

TECHNICAL DATA

Instruments	Purpose and Description
Solid State Physics	
4 Triple-axis Spectrometers	Inelastic scattering; diffuse scattering; powder diffractometer; polarized beam. Energy range: 2.5 meV $< E_o <$ 200 meV Q range: 0.03 $< Q <$ 10 $Å^{-1}$
Biology	
Small Angle Neutron Scattering	Studies of large molecules. Located on cold source with 20 × 20 cm^2 position-sensitive area detector. Sample detector distance L $<$ 2 meter Incident wavelength 4 Å $< \lambda_o <$ 10 Å
Diffractometer	Protein crystallography 20 × 20 cm^2 area detector λ_o = 1.57 Å
Chemistry	
2 Diffractometers	Single-crystal elastic scattering 4-circle goniometer 1.69 Å $< \lambda_o <$ 0.65 Å
1 Triple-axis Spectrometer	Inelastic scattering Diffuse scattering Powder diffractometry
Nuclear Physics	
3 Spectrometers	Neutron capture studies Energy range: 0.025 eV $< E_o <$ 25keV
TRISTAN II (Isotope Separator)	Spectroscopic study of neutron-rich unstable isotopes produced from U-235 fission
Irradiation Facilities	
7 Vertical Thimbles	Neutron activation; production of isotopes; thermal flux: 8.3x10^{14} neutrons/cm^2 sec; fast (>0.5 MeV) flux: 3×10^{14} neutrons/cm^2 sec.

NEUTRON SCATTERING AT THE HIGH FLUX ISOTOPE REACTOR

Solid State and Chemistry Divisions
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

The neutron scattering facilities at the High Flux Isotope Reactor (HFIR) are used for long-range basic research on the structure and dynamics of condensed matter. Active programs exist on the magnetic properties of matter, lattice dynamics, defect-phonon interactions, fluxoid lattices in superconductors, liquid structures, and crystal structures. The HFIR is a 100-MW, light-water moderated reactor with an unsurpassed record of operating time (better than 90%). The central flux is 5×10^{15} neutrons/cm^2 sec, and the flux at the inner end of the beam tubes is slightly greater than 10^{15} neutrons/cm^2 sec. A wide variety of neutron scattering instruments have been constructed with the support of the Division of Materials Sciences. Three of these are unique within this country: the triple-axis polarized-beam spectrometer, the double-crystal small-angle diffractometer, and the correlation chopper.

USER MODE

These facilities are open for use by outside scientists on problems of high scientific merit. Written proposals are reviewed for scientific feasibility by an internal review committee. It is expected that all accepted experiments will be scheduled within six months of the receipt of the proposal. No charges for the use of the beams will be assessed for research to be published in the open literature. The cost of extensive use of ORNL shop or computer facilities must be borne by the user. Travel and living expenses are also the user's responsibility. Inexperienced users will normally collaborate with an ORNL staff member. Proprietary experiments can be carried out after a contract has been arranged based on full cost recovery, including a charge for beam time. A brochure describing the facilities and a booklet giving user procedures are available on request.

PERSON TO CONTACT FOR INFORMATION

H. A. Mook
Solid State Division
Oak Ridge National Laboratory
Post Office Box X
Oak Ridge, Tennessee 37830

(615) 574-5242
FTS 624-5242

NEUTRON SCATTERING AT THE HIGH FLUX ISOTOPE REACTOR

TECHNICAL DATA

Beam No.	Instrument	Operating Characteristics
HB-1	Triple-axis polarized-beam	Beam size - 2.5 by 3 cm max. Flux - 2.6 x 10^6 neut/cm^2 sec at sample (polarized) Vertical magnetic fields to 5 T Horizontal fields to 2 T Variable E_o
HB-1A	Triple-axis, fixed E_o	E_o = 14.7 meV, 2.353 Å Beam size - 5 by 3.7 cm max. Flux - 9 x 10^6 neut/cm^2 sec at sample with 40' collimation
HB-2A	Liquid diffractometer with linear position sensitive detector	Beam size - 1 by 3.4 cm max. λ = 0.89 Å Flux - 6.8 x 10^5 neut/cm^2 sec at sample with 20' collimation
HB-2, HB-3	Triple-axis, variable E_o	Beam size - 5 by 3.7 cm max. Flux - 10^7 neut/cm^2 sec at sample with 40' collimation
HB-3A	Double-crystal small-angle diffractometer	Beam size - 4 x 2 cm max. Flux - 10^4 neut/cm^2 sec λ = 2.6 Å Resolution - 4 x 10^{-5} Å^{-1}
HB-4A	Four-circle diffractometer	Beam size - 5 x 5 mm Flux - 2 x 10^6 neut/cm^2 sec with 9' collimation λ = 1.015 Å
HB-4	Correlation chopper	Beam size - 5 x 3.7 cm Flight path - 1.5 m 70 detectors covering 130° Variable E_o Variable pulse width

INTENSE PULSED NEUTRON SOURCE (IPNS-I)

Argonne National Laboratory
Argonne, Illinois 60439

IPNS-I is an intermediate level pulsed spallation source dedicated to research on condensed matter. The peak thermal flux is about 3 x 10^{14} n/cm^2 sec. The source has some unique characteristics that promise to open up new scientific opportunities:

- high fluxes of epithermal neutrons (0.1-10 eV)
- pulsed nature, suitable for real-time studies and measurements under extreme environments
- very low gamma-ray backgrounds

Three principal types of scientific activity are underway at IPNS-I: neutron diffraction, concerned with the structural arrangement of atoms (and sometimes magnetic moments) in a material and the relation of this arrangement to its physical and chemical properties; inelastic neutron scattering, concerned with processes where the neutron exchanges energy and momentum with the system under study and thus probes the dynamics of the system at a microscopic level; and neutron radiation effects, concerned with the defect cascades produced in a material by a fast neutron radiation field and the effect of these cascades on its physical properties. At the same time, it is expected that the facilities will be used for fundamental physics measurements as well as for technological applications such as resonance neutron radiography.

USER MODE

IPNS is available without charge to qualified scientists doing fundamental research. Selection of experiments is made on the basis of scientific merit by a Program Committee consisting of eminent scientists, mostly from outside Argonne. Scientific proposals (2 pages long) are submitted twice a year and judged by the Program Committee. Full details, including a User's Handbook, Proposal and Experimental Report Forms, can be obtained from the Scientific Secretary, Dr. T. G. Worlton, IPNS-360, Argonne National Laboratory.

PERSONS TO CONTACT FOR INFORMATION

G. H. Lander, Program Director	(312) 972-5518 FTS 972-5518
B. S. Brown, Operations Manager	(312) 972-4999 FTS 972-4999
T. G. Worlton, Scientific Secretary	(312) 972-8755 FTS 972-8755

Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

INTENSE PULSED NEUTRON SOURCE (IPNS-I)

TECHNICAL DATA

NEUTRON SCATTERING

Facility (Instrument Scientist)	Assignment	Range		Resolution	
		†Wave-vector	Energy	Wave-vector	Energy
Special Environment Powder Diffractometer (J. D. Jorgensen)	F5	0.5-40 Å^{-1}	*	0.35%	*
General Purpose Powder Diffractometer (J. Faber, Jr.)	F2	0.5-100 Å^{-1}	*	0.25%	*
Single Crystal Diffractometer (A. J. Schultz)	H1	2-20 Å^{-1}	*	2%	*
Low-Resolution Medium-Energy Chopper Spectrometer (C.-K. Loong)	F4	0.1-30 Å^{-1}	0-0.6 eV	0.02 K_o	0.05 E_o
High-Resolution Medium-Energy Chopper Spectrometer (D. L. Price)	H3	0.3-9 Å^{-1}	0-0.4 eV	0.01 K_o	0.02 E_o
Small-Angle Scattering Diffractometer (J. E. Epperson (a), C. Borso (b))	C1	0.001- 0.3 Å^{-1}	*	0.004 Å^{-1}	*
Crystal Analyzer Spectrometer (T. O. Brun)	F1	3-16 Å^{-1}	0.02- 0.5 eV	3%	2%

* No energy analysis
† Wave-vector, $K = 4\pi \sin\theta/\lambda$
(a) Materials Science -- 3 Meter Flight Path
(b) Biology -- 8 Meter Flight Path

NEUTRON BEAMS AVAILABLE FOR SPECIAL EXPERIMENTS

Beam Tube	Current Use	Flight Path Length (m)
F3	eV Spectrometer	10
C2	Polarized Neutron Exp.	10
C3	Solid He^3 Project	10
F6	Irradiations	6-20
H2	Irradiations	6-20
V1	Ultra-Cold Neutron Exp.	4

RADIATION EFFECTS

Facility (Instrument Scientist)	Description
Radiation Effects Facility (R. C. Birtcher)	Two vertical (5 cm ID) tubes with flux 1 x 10^{12} n/cm^2 sec and one horizontal (3.8 cm ID) tube with flux 3 x 10^{11} for energy greater than 0.1 MeV at 8μA; capabilities for maintaining two samples at liquid helium temperature (4°K) and above

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SNR/PSR SPALLATION NEUTRON SOURCE

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

The SNR/PSR (Spallation Neutron Research/Proton Storage Ring) facility is a pulsed spallation neutron source driven by the 800-MeV Los Alamos Meson Physics (LAMPF) linear accelerator. Neutron scattering research is currently carried out at the WNR using the advantages of time-of-flight methods. Available instruments include: a) a general purpose powder diffractometer; b) a single crystal diffractometer based on the Laue-TOF technique; and c) a filter difference spectrometer for chemical and optic mode spectroscopy. A considerable effort is directed toward pulsed source instrument development including, currently, a constant Q spectrometer, a chopper spectrometer, an electron volt spectrometer, and a liquids and amorphous diffractometer. A proton storage ring (PSR) is under construction and by 1985 the SNR/PSR will provide at 12 neutron bursts per second the world's highest peak thermal flux for neutron scattering research. In addition, it will also be a source of epithermal neutrons many orders of magnitude larger than reactors for neutron scattering research in solid state physics, chemistry, biology, polymers, and materials science.

USER MODE

Two thirds of the neutron scattering beam time on user instruments at the WNR/PSR is allocated by a nationally appointed Program Advisory Committee. Application for instrument time can be made by submitting a completed proposal form for consideration by the PAC. The PAC evaluates proposals on the basis of scientific excellence and optimal use of SNR/PSR capabilities. One third of the neutron scattering beam time is reserved for Laboratory discretionary research, research pertinent to DOE applied program goals, and instrument development. The SNR/PSR instrumentation is available without charge for nonproprietary research. The facility is open to all U.S. citizens and permanent resident aliens, and to visits of less than seven working days for citizens of nonsensitive countries. DOE approval is required for any other foreign national visits.

PERSON TO CONTACT FOR INFORMATION

R.N. Silver
MS H805, Group P-8
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

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(FTS) 843-6069

SNR/PSR

TECHNICAL DATA

	1982	1985
Proton Source	LAMPF	LAMPF + PSR
Proton Source Current	750μA	1000μA
Proton Source Energy	800MeV	800MeV
SNR Proton Current	5μA	100μA
Proton Pulse Width	6μs	0.27μs
Repetition Rate	120Hz	12Hz
Epithermal Neutron Current (n/eV.Sr.S)	$1.6\times10^{11}/E$	$3.2\times10^{12}/E$
Peak Thermal Flux ($n/cm^2.S$)	5×10^{13}	1×10^{16}

User Instrument	Purpose and Description
General Purpose Powder Diffractometer	Liquids and amorphous metals, powder diffraction wave vector 0.3-50Å^{-1} resolution 0.45% powder 2% liquids
Single Crystal Diffractometer	Laue time-of-flight spectrometer wave vector 1-15Å^{-1} resolution 2% typical
Filter Difference Spectrometer	Inelastic neutron scattering, vibrational spectroscopy energy trans. 35-600 meV resolution 5-7%

NATIONAL CENTER FOR SMALL-ANGLE SCATTERING RESEARCH

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

The National Center for Small-Angle Scattering Research is supported by the National Science Foundation and the Department of Energy under an interagency agreement. The two main instruments available to users are the NSF-constructed 30-m small-angle neutron scattering facility (SANS) and the DOE-constructed 10-m small-angle x-ray scattering camera (SAXS). These instruments are intended to provide state-of-the-art capability for investigating structures of condensed matter on a global scale, e.g., from a few tens to several hundreds of angstroms. They are intended to serve the needs of scientists in the areas of biology, polymer science, chemistry, metallurgy and materials science, and solid state physics.

USER MODE

Beam time on these instruments is assigned, in general, on the basis of proposals submitted in advance. These are then reviewed by a panel of experts external to the Laboratory and are rated on the basis of scientific merit. When a favorable review has been received, a staff member of the NCSASR and the user agree, usually by telephone, on a time and duration for the experiment. Ordinary charges are borne by the Center, but extensive use of support facilities (shops, computing, etc.) must be paid by the user. Users may work in collaboration with one or more staff members if they wish, but such collaboration is not required. Proprietary experiments can be carried out after contractual agreement has been reached.

PERSONS TO CONTACT FOR INFORMATION

W. C. Koehler, Director NCSASR	(615) 574-5232	FTS: 624-5232
G. D. Wignall, SANS-NCSASR	(615) 574-5237	FTS: 624-5237
J. S. Lin, SAXS-NCSASR	(615) 574-4534	FTS: 624-4534
M. Gillespie, Secretary NCSASR	(615) 574-5231	FTS: 624-5231

Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

NATIONAL CENTER FOR SMALL-ANGLE SCATTERING RESEARCH

TECHNICAL DATA

30-m SANS Instrument Specifications

Monochromator: six pairs of pyrolytic graphite crystals

Incident wavelength: 4.75 Å or 2.38 Å

Wavelength resolution: $\Delta\lambda/\lambda = 6\%$

Source-to-sample distance: 10 m

Beam size at specimen: 0.5–3.0 cm diam

Sample-to-detector distance: 1.5–18.5 m

K range: $5 \times 10^{-3} \leq K \leq 0.6$ Å^{-1}

Detector: [illegible]4 by 64 cm^2

Flux at specimen: 10^4–10^6 neutrons cm^2 s^{-1} depending on slit sizes and wavelength

10-m SAXS Instrument Specifications

Monochromator: hot-pressed pyrolytic graphite

Incident wavelengths: 1.542 Å (CuK_α) or 0.707 Å (MoK_α)

Source-to-sample distances: 0.5, 1.0, 1.5. . . ., 5.0 m

Beam size at specimen: 0.1 by 0.1 cm (fixed)

Sample-to-detector distances: 1, 1.5, 2.0, ..., 5 m

K range covered: $3 \times 10^{-3} \leq K \leq 0.3$ Å^{-1} (CuK_α)
$6 \times 10^{-3} \leq K \leq 0.6$ Å^{-1} (MoK_α)

Maximum flux at specimen: 10^6 photons per second on sample-irradiated area 0.1 by 0.1 cm

Detector: 20- by 20-cm^2 (electronic resolution 0.1 by 0.1 cm^2)

Special features: deformation device for dynamic scattering experiments (time slicing in periods as short as 100 μs for oscillatory experiments or 10 s for transient relaxation experiments) and interactive graphics for data analysis

NATIONAL CENTER FOR ELECTRON MICROSCOPY

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

The National Center for Electron Microscopy (NCEM) was formally established in fall 1981 as a component of the Materials and Molecular Research Division, Lawrence Berkeley Laboratory.

The NCEM provides unique facilities and advanced research programs in the United States for electron microscopy characterization of materials. Its mission is to carry out fundamental research and maintain state-of-the-art facilities and expertise. Present instrumentation at the Center includes a conventional 650 kV Hitachi electron microscope installed in 1969 in the Hearst Mining Building on the University of California Berkeley campus, and a newly installed 1.5 MeV Kratos microscope dedicated largely for in-situ work, a 1 MeV JEOL atomic resolution microscope (ARM), and a high-resolution feeder microscope (JEOL 200CX). In late 1983, a 200 kV analytical microscope will be added. Facilities for image simulation, analysis, and interpretation will also be available to users.

USER MODE

Qualified microscopists with appropriate research projects of documented interest to DOE may use the Center without charge. Proprietary studies may be carried out on payment of full costs. Access to the Center may be obtained by submitting research proposals, which will be reviewed for Center justification by a Steering Committee (present external members are Drs. A. Simnad, Chairman; W. L. Bell, J. M. Gibson, D. A. Howitt, J. J. Hren, J. C. H. Spence, and A. Taylor; internal members are G. Thomas, R. M. Glaeser, R. Gronsky, and K. H. Westmacott). A limited number of studies judged by the Steering Committee to be of sufficient merit can be carried out as a collaborative effort between a Center postdoctoral fellow, the outside proposer and a member of the Center staff.

PERSON TO CONTACT FOR INFORMATION

Ms. Madeline Moore
National Center for Electron Microscopy
Mail Stop: 72-131
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

(415) 486-6062, or
FTS 451-6062

NATIONAL CENTER FOR ELECTRON MICROSCOPY

TECHNICAL DATA

Instruments	Key Features	Characterization
KRATOS 1.5 MeV Electron Microscope	Resolution 3Å (pt-pt) environmental cell; hot, cold stages	50-80 hrs/week 150-1500 kV range in 100 kV steps and continuously variable. Max beam current 70 amp/cm^2. 3 mm diameter specimens
JEOL 1 MeV Atomic Resolution Microscope (ARM) (available about August 1983)	Resolution ≤ 1.7Å (pt-pt) over full voltage range. Ultrahigh resolution goniometer stage, ± 40° biaxial tilt with height control	50-80 hrs/week 400 kV - 1 MeV LaB_6 filament 3 mm diameter specimens
Hitachi 650 kV Electron Microscope	General purpose resolution 20 Å environmental cell straining stage	Installed in 1969. Max. voltage 650 kV conventional HVE
JEOL 200 CX Electron Microscope	Dedicated high-resolution 2.4 Å (pt-pt) U.H. resolution goniometer stage only	200 kV only LaB_6 filament 2.3 mm diameter specimens
200 kV dedicated Analytical Electron Microscope (planned)	X-ray and energy-loss spectrometers microdiffraction (CEB)	100 kV - 200 kV state-of-the-art resolution

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HIGH VOLTAGE ELECTRON MICROSCOPE TANDEM FACILITY

Argonne National Laboratory
Argonne, Illinois 60439

The Argonne National Laboratory High Voltage Electron Microscope-Tandem Facility provides unique combinations of the techniques of high-voltage electron microscopy, ion implantation/bombardment, and ion-beam analysis.

The high-voltage electron microscope is an improved Kratos/AEI-EM7 with a maximum voltage of 1.2 MV, and a demonstrated lattice resolution of 3.5 Å. In addition to a 33° ion-beam access tube, the microscope contains a number of specialized features. These include a negative ion trap, an ion-pumped specimen chamber, two independently adjustable dark-field conditions, a 100-1200 kV continuous-mode voltage selection from the control desk, and a beam dosimetry system for both the ion and the electron beams. A variety of side entry single and double tilt stages are available, which permit observations between 10 and 1000 K in vacuo, and from ambient to 1300 K in gaseous environments. Two straining stages are also available for work either in vacuo or in the environmental cell. The ANL HVEM is equipped with a Harwell design camera, and a Cohu video camera and image intensifer are mounted beneath the microscope column.

A National Electrostatics 2 MV Tandem Ion Accelerator and a 300 KV ion accelerator together can produce ion beams from 10 keV to 8 MeV of most stable elements in the periodic table. The tandem unit has two external negative ion sources and a positive ion source in the terminal. Ions from the accelerators can be transported into the microscope through the "ion-beam interface" to permit direct observation of the effects of ions as well as electron bombardment on materials in the HVEM.

USER MODE

The HVEM-Tandem facility is operated as a national materials science resource. Qualified scientists wishing to conduct experiments should submit a proposal to the person named below. Decisions as to which experiments will be done are made by a Program Advisory Committee following peer evaluation of the proposals. There are no use charges for users carrying out basic research of documented interest to DOE. Use charges will be levied for proprietary investigations.

PERSON TO CONTACT FOR INFORMATION

A. Taylor
Manager, HVEM-Tandem Facility
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

(312) 972-5109
FTS 972-5109

ARGONNE NATIONAL LABORATORY HIGH VOLTAGE ELECTRON MICROSCOPE-TANDEM FACILITY

TECHNICAL DATA

Instrument	Key Features
KRATOS 1.2 MeV Electron Microscope	Resolution 3,5 Å lattice Magnification 63-1,000,000X Continuous voltage selection Current density 15 A/cm^2 High-vacuum specimen chamber Two switched dark field conditions Negative ion trap Electron dosimetry system Cohu video system Ion beam access port Cryogenic anticontaminator
Accelerators	
NEC Model 2 UDHS	Terminal voltage - 2 MV Energy stability - ±250 eV Current density - H^+ 10 $\mu A/cm^2$ (typical) Ni^+ 1 Pt^+ 0.1
Texas Nuclear 300-kV	Terminal voltage - 300 kV Energy stability - ±300 eV Current density - H^+ 20 $\mu A/cm^2$ (typical) Ni^+ 2 Pt^+ 2
Ion Sources	Available for both accelerators: Danfysik 910, 911 Sputter Duoplasmatron External for tandem: Alphatros SNICS
Ion Beams	Any stable isotope
Beam Lines	Ion-beam interface to HVEM Beamlines and target chambers for irradiation and in beam analysis Dual-ion target chamber

SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

Metals and Ceramics Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

The microanalysis facilities for use in materials science have been made available for collaborative research by members of universities or industry with ORNL staff members. The facilities include state-of-the-art analytical transmission electron microscopy, high voltage electron microscopy, surface analysis, and nuclear microanalysis. The electron microscopy capabilities include high resolution, high voltage, and analytical (energy dispersive x-ray spectroscopy and electron energy loss spectroscopy). Surface analysis facilities include four Auger electron spectroscopy (AES) systems; ion backscattering and nuclear reaction techniques using the 0.4 and 5.0 MV Van de Graaff accelerators in the Metals and Ceramics Division.

USER MODE

User interactions are through collaborative research projects between users and researchers on the Materials Sciences Program at ORNL. Proposals are reviewed by an executive committee which consists of ORAU, ORNL, and university members. Proposals are evaluated on the basis of scientific excellence and relevance to DOE needs and must identify one ORNL staff member who will share responsibility for the project.

The SHaRE program provides technical help and limited travel expenses for academic participants through the Oak Ridge Associated Universities (ORAU).

PERSONS TO CONTACT FOR INFORMATION

E. A. Kenik (615) 574-5066
Metals and Ceramics Division FTS 624-5066
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

A. Wohlpart (615) 576-3422
Oak Ridge Associated Universities FTS 626-3422
P.O. Box 117
Oak Ridge, Tennessee 37830

SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

Technical Data

Instruments and Facilities	Key Feature	Operating Characteristics
Hitachi HU-1000 High Voltage Electron Microscope	Heating stages; in situ deformation stages; low light level videorecording system; environmental cell — 0-1 atm	0.3-1.0 MeV; electron irradiation studies; ten 4-h shifts/week; available evenings, weekends to qualified users
Philips EM400T/FEG Analytical Electron Microscope	TEM resolution <0.16 nm; STEM resolution <1.0 nm; energy dispersive x-ray analysis; electron energy loss spectroscopy; convergent beam electron diffraction	120 kV; ten 4-h shifts/week; available evenings, weekends, to qualified users; structural and elemental microanalysis; minimum probe diameter <1 nm
JEOL 120CX Analytical Electron Microscope	TEM resolution ~0.34 nm; STEM resolution ~3 nm; energy dispersive x-ray analysis; electron energy loss spectroscopy	120 kV; ten 4-h shifts/week; structural and elemental microanalysis; minimum probe diameter <10 nm
JEOL 120C Transmission Electron Microscope	TEM resolution ~0.34 nm; special polepiece for TEM of ferromagnetic materials	120 kV; ten 4-h shifts/week; structural microanalysis
PHI 590 Scanning Auger Electron Spectroscopy System	200 nm beam size; fracture stage; residual gas analysis; sputter depth profiling; elemental mapping	Surface analytical and segregation studies
Varian Scanning Auger Electron Spectroscopy System	5 µm beam size; hot-cold fracture stage; residual gas analysis; sputter depth profiling; elemental mapping	Surface analytical and segregation studies; gas-solid interaction studies
Dual Ion-Beam Accelerator Facilities	4 MW Van de Graaff accelerator; 400 kV accelerator; sputter depth profiling	Nuclear microanalysis; Rutherford backscattering; elemental analysis

CENTER FOR MICROANALYSIS OF MATERIALS

Materials Research Laboratory
University of Illinois
Urbana-Champaign, Illinois 61801

The Center operates a wide range of advanced surface chemistry and electron-beam microanalytical equipment for the benefit of the University of Illinois materials research community and for the DOE Laboratories and Universities Programs. Equipment is selected to provide a spectrum of advanced microcharacterization techniques including microchemistry, microcrystallography, surface analysis, etc. A team of professionals runs the facility and its members facilitate the research.

USER MODE

Most of the research in the facility is funded by MRL contracts of the University of Illinois faculty, and is carried out by graduate students, post-doctoral and faculty researchers and by the Center's own professional staff.

For the benefit of external users the system retains as much flexibility as possible. The preferred form of external usage is collaborative research through a contract with a faculty member associated with the MRL, or by direct negotiation with the management of the Center. Direct user access to the equipment is also possible, for trained individuals. In all cases, the research carried out by facility users has to be in the furtherance of DOE objectives.

The facility staff maintain training programs in the use of the equipment and teach associated techniques. An increasing part of the Center's activity is concerned with the development of new instruments and instrumentation.

A brochure describing the Center and its services is available.

PERSON TO CONTACT FOR INFORMATION

Dr. J. A. Eades, Coordinator (217)-333-8396
Center for Microanalysis of Materials
Materials Research Laboratory
University of Illinois
104 S. Goodwin
Urbana, Illinois 61801

CENTER FOR MICROANALYSIS OF MATERIALS

Instruments

Imaging Secondary Ion Microprobe Cameca IMS 3f	Mass analysed images to 0.3μ res. Positive and negative ions.
Scanning Auger Microprobe Physical Electronics 595	Resolution: SEM 300 Å, Auger 700 Å. Windowless X-ray detector.
Scanning Auger Microprobe Physical Electronics 545	Resolution: SEM 3μ. Specimen temp: 77-600 K.
XPS Physical Electronics 548	Double pass CMA. ESCA and Auger analysis. Specimen temp. to 1550 K.
Transmission Electron Microscope Philips EM420 (120kV)	EDS, EELS, STEM. Cold stage (30K). Computer Control.
Transmission Electron Microscope Philips EM400T (120kV)	EDS. Heating, cooling stages.
Scanning Transmission Electron Microscope Vacuum Generators HB 5 (35kV)	5Å probe, EDX, EELS.
Scanning Electron Microscope JEOL JSM 35C (35kV)	50Å resolution, EDX.
Rutherford Backscattering (in-house construction) (3 MeV)	Under development
X-ray Equipment Elliott 14 kW high brilliance source Rigaku 12 kW source Several Conventional Sources	4-circle diffractometer. Small angle camera. EXAFS. Lang topography. Powder cameras, etc.
Transmission Electron Microscope (300 kV)	Delivery winter 1983/1984

In addition to the main items listed above the Center also has other equipment: a second scanning electron microscope, two electron microprobes, a spark source mass spectrometer, optical microscopes, a surface profiler, a microhardness tester, etc. Dark rooms and full specimen preparation facilities are available, including five ion-milling stations, evaporators, electropolishing units, sputter coaters, a spark cutter, an acid saw, etc.

The equipment is made available on a flexible week-by-week booking scheme; if professional help is required, operating hours at 8-5, except by special arrangement. Fully qualified users can and do use the equipment at any time of day. Several of the instruments are maintained in almost continuous (24 hour) use.

SURFACE MODIFICATION AND CHARACTERIZATION COLLABORATIVE RESEARCH CENTER

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

This program utilizes a new approach for fundamental materials research. The combined techniques of ion implantation doping, ion-induced mixing and pulsed-laser processing are utilized to alter the near-surface properties of a wide range of solids in ultrahigh vacuum. Through in situ analysis by ion beam, surface, and bulk properties techniques, the fundamental materials interactions leading to these property changes are determined. Since both ion implantation doping and pulsed-laser annealing are nonequilibrium processing techniques, they can be used to produce new and often unique materials properties not possible with equilibrium fabrication techniques. This makes them ideal tools for fundamental materials research. They are equally useful for modifying surface properties for practical applications in areas such as friction, wear, corrosion, catalysis, surface hardness, solar cells, semiconducting devices, superconductors, etc.

This program has emphasis on long-range basic research. Consequently, most collaborative research involving scientists from industries, universities, and other laboratories has been the investigation of new materials properties possible with these processing techniques or the determination of the mechanisms responsible for observed property changes. In most instances such research projects identify definite practical applications and accelerate the transfer of these materials alteration techniques to processing applications.

COLLABORATIVE RESEARCH

User interactions are through mutually agreeable collaborative research projects between users and research scientists at ORNL which utilize the unique alteration/analysis capabilities of the SMAC facility. Because of the tremendous interests expressed in these techniques and the broad range of existing collaborations, plans for a users' facility have been initiated. Until this program has been established, the informal arrangement will be continued. It should be emphasized that the goal of these interactions is to demonstrate the usefulness or feasibility of these techniques for a particular materials application and not to provide routine service alterations or analyses.

PERSON TO CONTACT FOR INFORMATION

B. R. Appleton (615) 574-6283
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Oak Ridge National Laboratory
Post Office Box X
Oak Ridge, Tennessee 37830

SURFACE MODIFICATION AND CHARACTERIZATION COLLABORATIVE RESEARCH CENTER

TECHNICAL DATA

Accelerators	Operating Characteristics
2.5-MV Positive Ion Van de Graaff	0.1–3.2 MeV; H, D, ^{4}He, ^{3}He, and selected gases. Beam current ∿50 μamps.
10–200-KV High-Current Ion Implantation Accelerator	Essentially any species of ion. 1–10 mamps singly charged, ∿100 μamps doubly and triply charged.
0.1–10-KeV Ion Gun	Gaseous species. ∿100 μamp.
Lasers	
Pulsed Ruby Laser (0.6943 μm)	15–30 x 10^{-9} s pulse duration time. 10 Joule/Pulse Output Multimode, 2-1/2 Joule/Pulse Output Single Mode (TEM_{00}).
Pulsed Ruby Laser (0.6943 μm)	15–30 x 10^{-9} s pulse duration time. 8 Joule/Pulse Output Single Mode (TEM_{00}).
Pulsed Nd:YAG/Glass Laser Wavelengths: 1.06 μm, 0.530 μm, 0.353 μm, 0.265 μm	15 x 10^{-9} s. 20 Joule/Pulse (1.06 μm), 5 Joule/Pulse (0.530 μm), 1 Joule/Pulse (0.265 μm). 30,50,100 or 200 x 10^{-12} s. 0.7 Joule/Pulse (1.06 μm) 0.2 Joule/Pulse (0.530 μm), 0.07 Joule/Pulse (0.265 μm).
Pulsed Excimer Laser (0.308 μm)	20 x 10^{-9} s. 1.5 Joule/Pulse.
Facilities	
UHV Surface and Near-Surface Analysis Chambers	Several chambers. Vacuums 10^{-6}–10^{-11} Torr. Multiple access ports. Liquid helium cryostat, UHV goniometers (4–1300 K).
In Situ Analysis Capabilities	Ion scattering, ion channeling, ion-induced nuclear reactions and characteristic X rays. LEED, Auger, ion-induced Auger. Optical emissions from sputtered particles. Laser fluorescence spectroscopy. Electrical resistivity vs temperature.
Combined Ion-Beam and Laser Processing	Laser and ion beams integrated into same UHV chambers.
Dual Simultaneous Ion-Beam Irradiations	Combined accelerator irradiations.

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COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

Sandia National Laboratories
Livermore, California 94550

Optical diagnostics, primarily spontaneous Raman spectroscopy, are being developed and used to study high temperature corrosion and erosion of materials for combustion systems. Emphasis is on the use of these techniques to identify chemical compounds present on surfaces during attack in hostile environments. In-situ analyses can be obtained with excellent temporal resolution (approximately 10 spectra per second) from samples in high temperature corrosive environments. Both pulsed and continuous lasers at various wavelengths throughout the visible and ultraviolet are available for excitation of Raman scattering, which can be detected using photon counting, gated integration, or optical multichannel techniques. These measurements are complemented by post-exposure Raman measurements including a Raman microprobe which allows analysis with micron spatial resolution. Other techniques including Sputter Induced Photon Spectroscopy (SIPS), Scanning Auger Microscopy (SAM), X-ray diffraction, and metallographic analysis provide complementary compositional and morphological information. Present research concerns include oxidation-sulfidation of Fe-Cr and Fe-Mn-Al alloys, chemical attack of stabilized zirconia thermal barrier coatings, corrosion of ion-implanted metals, and combined oxidation-erosion of steel. The goal is to obtain information about attack mechanisms utilizing data obtained during the corrosion processes.

Equipment which is available in a collaborative mode also includes the atmospheric combustor exhaust simulator (ACES) which produces an environment for realistic corrosion/erosion studies with capability for in-situ Raman analysis. ACES provides a high velocity (50 feet per second), high temperature (1000°C) gas flow with provision for particulate injection. This apparatus is being used for in-situ Raman studies and for erosion experiments.

USER MODE

This materials program at Sandia has emphasized research into corrosion and erosion mechanisms using the techniques and equipment described above. Interactions include collaborative research projects with outside users and providing information on new diagnostic approaches to the study of corrosion. In initiating collaborative research projects it is generally desirable to perform preliminary Raman analyses of typical samples and of reference materials to determine sensitivity to expected corrosion products. Subsequently, a brief written proposal is requested. Generally, visits of a week or more for external users provide an optimum period for information exchange and joint research efforts. Users from industrial, university, and government labs have been involved in these collaborative efforts. Results of these research efforts are published in the open literature.

PERSON TO CONTACT FOR INFORMATION

Richard E. Palmer
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Sandia National Laboratories
Livermore, California 94550

(415)422-3126
FTS 532-3126

COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

TECHNICAL DATA

Instruments	Key Features
Raman Spectrometer	Rejects elastic light to within 50 cm^{-1} of laser line. 100 ms. temporal resolution.
Raman Microprobe	1 micron spatial resolution.
Sputter Induced Photon Spectroscopy (SIPS)	5 keV argon beam surface analysis of insulators.
Atmospheric Combustor Exhaust Simulator	50 fps flow 1000°C temperature Particulate injection

MATERIALS PREPARATION CENTER

Ames Laboratory
Iowa State University
Ames, Iowa 50011

The Materials Preparation Center was established because of the unique capabilities for preparation, purification, fabrication and characterization of certain metals and materials that have been developed by investigators at the Ames Laboratory during the course of their basic research. Individuals within the Laboratory's Metallurgy and Ceramics Program are widely recognized for their work with very pure rare-earth, alkaline-earth and refractory metals. Besides strengthening materials research and development at the Ames Laboratory, the Center increases awareness by the research community of the scope and accessibility of this resource to universities, other government and private laboratories and provides appropriate transfer of unique technologies developed at the Center to private, commercial organizations.

Through these research efforts at Ames, scientists are now able to acquire very high-purity metals and alloys in single and polycrystalline forms, as well as the sophisticated technology necessary to satisfy many needs for special preparations of rare-earth, alkaline-earth, refractory and some actinide metals. The materials in the form and/or purity are not available from commercial suppliers, and through its activities the Center helps assure the research community access to materials of the highest possible quality for their research programs.

The Center consists of a Materials Preparation Section, an Analytical Section and the Materials Referral System and Hotline (MRSH). The Analytical Section has extensive expertise and capabilities for the characterization of materials, including complete facilities for chemical and spectrographic analyses, and selected services of this section are available to the research community. The purpose of MRSH is to accumulate information from all known National Laboratory sources regarding the preparation and characterization of materials and to make this information available to the scientific community.

USER MODE

Materials Preparation and Analytical Sections

Quantities of ultrapure rare-earth metals and alloys in single and polycrystalline forms are available. Special preparations of high-purity oxides and compounds are also available in limited quantities. Unique technologies developed at Ames Laboratory are used to prepare refractory metals in single and polycrystalline forms. In addition, certain alkaline-earth metals used as reducing agents are available. Complete characterization of these materials are provided by the Analytical Section. Materials availability and characterization information can be obtained from Frederick A. Schmidt, Director, Materials Preparation Center.

Materials Referral System and Hotline

The services of the Materials Referral System are available to the scientific community and inquires should be directed to Tom Wessels, MRSH Manager, (515) 294-8900 or FTS 865-8900.

TECHNICAL DATA

Materials

Scandium
Yttrium
Lanthanum
Cerium
Praseodymium
Neodymium
Samarium
Europium
Gadolinium
Terbium
Dysprosium
Holmium
Erbium
Thulium
Ytterbium
Lutetium

Titanium
Vanadium
Chromium
Manganese
Zirconium
Niobium
Molybdenum
Hafnium
Tantalum
Tungsten

Magnesium
Calcium
Strontium
Barium

Thorium
Uranium

PERSON TO CONTACT FOR INFORMATION

Frederick A. Schmidt, Director (515) 294-5236
Materials Preparation Center FTS 865-5236
121 Metals Development Building
Ames Laboratory
Ames, Iowa 50011

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LOS ALAMOS EQUATION OF STATE LIBRARY CENTER*

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

The Los Alamos Equation of State (EOS) Library is a computer-based library of EOS data and FORTRAN subroutines developed at Los Alamos. It is used nationally and internationally by many Laboratories, universities, research institutes and private corporations. The Library is becoming a standard reference resource for EOS and related data.

The Library contains EOS tables of pressure and internal energy as functions of temperature and density for approximately 50 different materials. The tabular format has several advantages: (1) it can represent phase transitions accurately, (2) it covers a wide range of temperatures and densities, and (3) it is easily updated to incorporate new experimental or theoretical results in specific regions of temperature and density. All types of materials are tabulated, including gases, metals, ceramics, plastics, glasses, and even composites such as rocks and minerals.

The associated subroutine library contains programs to update and retrieve data for a given material as well as accurate interpolation schemes for that data. These subroutines can be used directly in the user's computer program and have been incorporated in a number of Lagrangian and Eulerian fluid dynamic codes. The tables are sent from Los Alamos to other institutions on magnetic tapes, in a format that can be interpreted even if the other installation has a computing system different from that at Los Alamos. In most cases, the user can begin to apply the new table to a problem without having to analyze, interpret, or adapt it to his particular needs. Information about the availability of new data is communicated to users by journal articles, reports, informal newsletters, and by personal contact.

The EOS tables usually cover a much wider range of pressure and temperature than can be studied by experimental methds. To construct the tables, it is necessary to employ theoretical models of solids, liquids, vapors, and plasmas, for mixtures and chemical compounds as well as pure elements. EOS tables of high standard from sources other than Los Alamos, even though of more restricted pressure-temperature ranges, are also incorporated in the Library. Other related material properties, such as radiative opacities and conductivities, are available.

USER MODE

The Los Alamos EOS Library is available to users free of charge. To obtain the Los Alamos EOS Library, a user should send a list of materials required and two magnetic tapes with write format specification to

SESAME Library, T-4, MS B212
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

PERSON TO CONTACT FOR INFORMATION

Stanford P. Lyon
MS B212
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

(505) 667-7024
(FTS) 843-7024

LOS ALAMOS EQUATION OF STATE LIBRARY

TECHNICAL DATA

Materials

Air (dry)
Alumina (Al_2O_3)
Aluminum
+ Ammonia
Argon

Beryllium
Boron carbide
Brass
+ Butane (normal)

+ Calcium carbonate
Carbon (liquid)
Carbon phenolic
Copper

Deuterium
+ Deuterium-tritium mixture
+ Deutero-polyethylene
Diamond

Granite (Westerly)
Gold

Helium
High explosive
Hydrogen

Iron

Krypton

Lead
Lithia-boria glass
Lithium
Lithium deuteride
Lithium hydride

Mica
Methane
Molybdenum

Neon
Nevada alluvium
Nickel
Nitrogen
Oxygen

PBX-9502 (explosive)
Platinum
+ Polyethylene (branched)
+ Polyethylene (linear)
Polystyrene
+ Polytetraflouroethylene
Polyurethane

Quartz (SiO_2)

Ross-Aller solar mix

Sodium
Sodium chloride
Stainless steel

+ Tantalum
Tungsten carbide

Uranium
Uranium dioxide

Water

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*The EOS library is a unique source of data that is utilized internationally. Although it is not a facility research center as others listed in this section, it is included for information purposes.

+Equations of state for these materials were added in the last 12 months.

SECTION E

Summary of
Funding Levels

SUMMARY OF
FUNDING LEVELS

During the fiscal year ending September 30, 1983, the Materials Sciences total support level amounted to about $108.7 million in operating funds (budget outlays) and $8.5 million in equipment funds. The following analysis of costs is concerned only with operating funds i.e., equipment funds which are expended primarily at Laboratories are not shown in the analysis. In contrast, equipment support for the Contract Research projects is included as part of the operating budget.

1. By Region of the Country:

	Contract Research (% by $)	Total Program (% by $)
(a) Northeast................ (Mass., Penn., N.Y., N.J., Del., D.C., Md., Vt., Conn., Me., N.H., R.I.)	47.8	27.8
(b) South.................... (Fla., N.C., Tenn., Va., La., Ga., Ky., W.Va.)	9.5	19.6
(c) Midwest.................. (Ohio, Ill., Wisc., Mich., Mo., Minn., Ind., Iowa, Kan.)	19.4	31.0
(d) West..................... (Ariz., Okla., Wash., Texas, N.Mex., Calif., Utah, Colo., Idaho)	23.3	21.6
	100.0	100.0

2. By Academic Department or Laboratory Division:

	Contract Research (% by $)	Total Program (% by $)
(a) Metallurgy, Materials Science, Ceramics (Office Budget Activity Numbers 01-).............	63.8	40.4
(b) Physics, Solid State Science, Solid State Physics (Office Budget Activity Numbers 02-)....	30.8	49.2

	Contract Research (% by $)	Total Program (% by $)
(c) Chemistry, Chemical Eng. (Office Budget Activity Numbers 03-).............	5.4	10.4
	100.0	100.0

3. By University, DOE Laboratory, and Industry:

	Total Program (% by $)
(a) University Programs (including laboratories where graduate students are involved in research to a large extent, LBL, Ames)..................	33.6
(b) DOE Laboratory Programs.............	65.6
(c) Industry and Other..................	0.8
	100.0

4. By Laboratory and Contract Research:

	Total Program (%)
Ames Laboratory	6.6
Argonne National Laboratory	18.4
Brookhaven National Laboratory	19.1
Idaho National Engineering Laboratory	0.4
Illinois, University of (Materials Research Laboratory)	2.7
Lawrence Berkeley Laboratory	7.3
Lawrence Livermore National Laboratory	1.3
Los Alamos National Laboratory	3.4
Oak Ridge National Laboratory	18.0
Pacific Northwest Laboratory	1.8
Sandia National Laboratories	3.0
Solar Energy Research Institute	0.3
Contract Research	17.7
	100.0

5. By Selected Areas of Research:

	% of Projects[a] (Total=398)	% of Program Funding[a] ($108.7 million)
Materials		
Ceramics (Crystalline)	31	13.1
Ferrous Alloys	19	7.0
Intermetallics/Hydrides	13	4.9
Polymers	9	2.3
Semiconductors	14	6.3
Technique		
Electron Microscopy (Technique Development)	10	4.0
Neutron Scattering	10	17.7
Synchrotron	8	10.6
Theory	32	9.8
Phenomena		
Catalysis	6	2.4
Corrosion	11	6.4
Diffusion	13	4.0
Processing Science/Synthesis[b]	34	14.8
Strength	12	8.2
Superconductivity	9	4.3
Environment		
High Temperature (> 1200°K)	8	4.8
Radiation	12	13.7
Sulfur-Containing Gases	3	2.1

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[a] The summary funding levels for various research categories were determined from the index listing in Section F and estimating the percentage from the project devoted to a particular subject. There is overlap in the figures. For instance, funding for a project addressing creep of oxides would appear in the categories of ceramics, strength, and (possibly) high temperature.

[b] Based on projects indexed in Section F under coatings, materials preparation, powder metallurgy, solidification, surface treatments, thin films, and welding.

SECTION F

Index of Investigators, Materials, Techniques, Phenomena and Environment

The following indexes refer to project numbers in Sections A, B and C.

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